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SOLUBILITY DATA SERIES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: Hydrocarbons C8 to C36

SOLUBILITY DATA SERIES

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Editor-in-Chief A.S. KERTES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: Hydrocarbons C₈ to C₃₆

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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. 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 all 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 disqualified as such. In fact, it is only when the reliable data are 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.

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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, formulated at the initiation of the project and perfected as experience has accumulated, 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 the early 1970s to refrain from unnecessary publication has not achieved much. A good fraction of the literature is still 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 presents solubility data for binary systems in which one component is a hydrocarbon containing 8 to 36 carbon atoms and the second component is water, heavy water or seawater. Other volumes in this series either presently available or in preparation present analogous data for other hydrocarbons. The interested reader should consult the Solubility Data Series list of volume titles on page 561. For this volume seawater has been defined as, "all natural waters, synthetic seawater and aqueous solutions in which sodium chloride predominates."

A variety of units for the expression of solubility has appeared in the primary literature. For the purpose of comparison the compilers of this volume have, so far as possible, expressed all original results in terms of mass percent and mole fraction as well as the units presented by the original investigators. Where such conversions have been made, they are clearly attributed to the compiler and the source of any data not provided by the original investigators (such as hydrocarbon or seawater density) is specified. Definitions of mass percent and mole fraction as well as their relationship to other common measures of solubility are given in the Introduction to this volume.

The expression of the solubility of a hydrocarbon in natural seawater on a mole fraction basis presents special difficulties since the composition of seawater is not fully known and somewhat variable. However, the uncertainty introduced by this factor is generally less than 3%, smaller than the measurement uncertainty associated with many of these data. Some of the data for hydrocarbon solubility in seawater have been presented in terms of the Setschenow (also transliterated Sechenov and Setchenoff) equation. A thorough discussion, "The Sechenov Salt Effect Parameter", is presented in Volume 10 of this series (pp. xxix-xliii).

By far the most common approach to the measurement of solubility in hydrocarbon/water systems has been to prepare a saturated solution and then to analytically determine the concentration of the less abundant component. In these systems of low solubility the careful preparation of saturated solutions is critically important. The presence of only a small amount of the minor component in the form of colloidal droplets can significantly influence the solubility results obtained. This can lead to major positive systematic errors. Unfortunately, lack of experimental detail in some published reports makes these errors extremely difficult to evaluate. Users of this volume are advised to be aware of this potential source of error, especially for systems where only one or a few measurements have been reported or when solubilities are very low. Another approach to evaluating solubility data in these systems is to determine whether a particular result fits into a "reasonable" trend for a series of related compounds. While this approach undoubtedly has qualitative value, it must be used with caution. For instance, the solubilities of anthracene and phenanthrene differ by about a factor of 20; a fact that is supported by careful experimentation but not by "reasonable" inference.

Most measurements of hydrocarbon/water solubility have been made within the temperature range considered "room temperature" (275-300 K). In many reports system pressure is unspecified but can be assumed to be approximately 100 kPa (1 atm). Some measurements at elevated temperatures have been in sealed tubes. Generally the system pressure for these measurements is not known. For most purposes this lack of specification of system pressure is not important since hydrocarbon/water solubilities do not vary strongly with pressure.

This volume is the result of a careful search of the chemical literature. The goal of that search was to include all published data for the systems indicated in the title. Each evaluation includes a closing date for the literature search of that system, November 1981 or later. In spite of these efforts, some published measurements may have been missed. The editor will appreciate having his attention brought to any omitted source of solubility data for inclusion in future volumes.

The compilation and critical evaluation of solubility data presented here was a group effort. Each participant brought an individual style to the work. The editor's goal was to ensure that all text is simple, unambiguous English; not to attempt stylistic uniformity. Finally the editor wishes to acknowledge the dedicated efforts of the compilers, evaluators and reviewers whose efforts have resulted in this volume, and especially to thank Mauricette Nicpon, Sheila Chapin and Bronwyn Airey for final typing.

David Shaw

INTRODUCTION TO THE SOLUBILITY OF LIQUIDS IN LIQUIDS

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", "doubtful" 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.

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, with no distinction being made between solvent and solute.

The *solubility* of a substance 1 is the relative proportion of 1 in a mixture which is saturated with respect to component 1 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):

$$x_{1} = n_{1} / \sum_{i=1}^{n} i = \frac{m_{1} / M_{1}}{\sum_{i=1}^{n} (m_{i} / M_{i})}$$

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.

<u>Mole per cent</u> of component 1 is $100x_1$.

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

$$w_1 = m_1 / \sum_i m_i$$

where m_i is the mass of component *i*.

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

$$x_{1} = \frac{\frac{w_{1}/M_{1}}{w_{1}/M_{1} + (1 - w_{1})/M_{2}}}{\frac{w_{1}}{M_{1} + (1 - w_{1})/M_{2}}}$$

<u>Amount-of-substance concentration</u> of component 1 in a solution of volume V,

$$c_1 = n_1 / v$$

is expressed in units of mol dm^{-3} . 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 "part per million" (ppm) is not used, but may be expressed as $mg(1)/kg \ sln$.

<u>Molality</u> of component 1 in component 2 is often used in solid-liquid systems, defined $m_1 = n_1/n_2 M_2$, with units mol kg⁻¹, 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 unit (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 (e.g. cycloalkene, diene, alkyne, cycloalkane, alkane), 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 of substitution, then
- (vi) alphabetically by IUPAC name.

For example,

с ₅ н ₈	cyclopentene 2-methyl-1,3-butadiene 1,4-pentadiene 1-pentyne
C ₅ H ₁₀	cyclopentane 3-methyl-1-butene 2-methyl-2-butene 1-pentene 2-pentene
C ₅ ^H 12	2,2-dimethylpropane 2-methylbutane pentane
с ₅ н ₁₂ о	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

Introduction

C₆H₁₂0 cyclohexanol 4-methyl-1-penten-3-ol 1-hexen-3-ol 4-hexen-3-ol C₁₈H₁₂ benzanthracene chrysene naphthacene triphenylene

Deuterated compounds immediately follow the corresponding ¹H 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 IUPAC name (ref 1), chemical formula according to the Hill system, and Chemical Abstracts Registry Number. Also included are trivial name or names if appropriate.

"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).

"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 authors'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 percent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref 5) are used in such calculations. When appropriate, conversions from concentrations to mole fractions are included in the compilation sheets, 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.

"Method". An outline of the method is presented, reference being made to sources of further detail if 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) or (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 (identified by "compiler" in parentheses) from the internal consistency, the type of apparatus, and other relevant information. Methods used by the compilers for reporting estimating 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 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) 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 is rejected, the reference being included in the evaluation together with a reason for its rejection by the evaluator.

(d) *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.

(e) Units. The final recommended values are reported in SI units (ref 3).

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

- Rigaudy, J.; Klesney, S.P. Nomenclature of Organic Chemistry (IUPAC), ("The Blue Book"), Pergamon, Oxford, <u>1979</u>.
- 2. Hill, E.A. J. Am. Chem. Soc. 1900, 22, 478.
- 3. Whiffen, D.H., ed. Manual of Symbols and Terminology for Physicochemical Quantities and Units (IUPAC), ("The Green Book"), Pergamon, Oxford, <u>1979</u>; 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 Weight, Pure Appl. Chem. <u>1976</u>, 47, 75; <u>1979</u>, 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>.

THE PHASE BEHAVIOR OF WATER AND HYDROCARBON SYSTEMS

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In order to understand solubility in hydrocarbon + water systems at high pressure it is desirable to be aware of the various types of fluid phase equilibria possible in binary mixtures. Fluid phase equilibria of binary mixtures are conveniently discussed in terms of the classification proposed by Scott and van Konynenburg¹⁻⁴. They proposed that the phase behavior of binary mixtures could be classified into six broad groups. They found that five groups could be predicted using the van der Waals equation of state. The sixth class, which could not be predicted by the van der Waals equation, arises only in aqueous mixtures. The classification is most easily understood in terms of the pressure-temperature projection of the pressure-temperature-composition diagram. The six types of phase behavior are represented schematically in fig. 1. Only the "general" characteristics of the type of phase behavior can be understood from the diagrams given below. In practice solid phases often complicate the diagrams.

Type I. The phase diagram has a simple continuous gas-liquid critical locus with or without azeotropy.

Type II. The phase diagram is as for type I but with the addition of a three phase (liquid-liquid-gas) line ending at an upper critical end point, UCEP, and a (liquid-liquid) critical line starting from the UCEP and rapidly approaching high pressures. This type can occur with or without azeotropy.

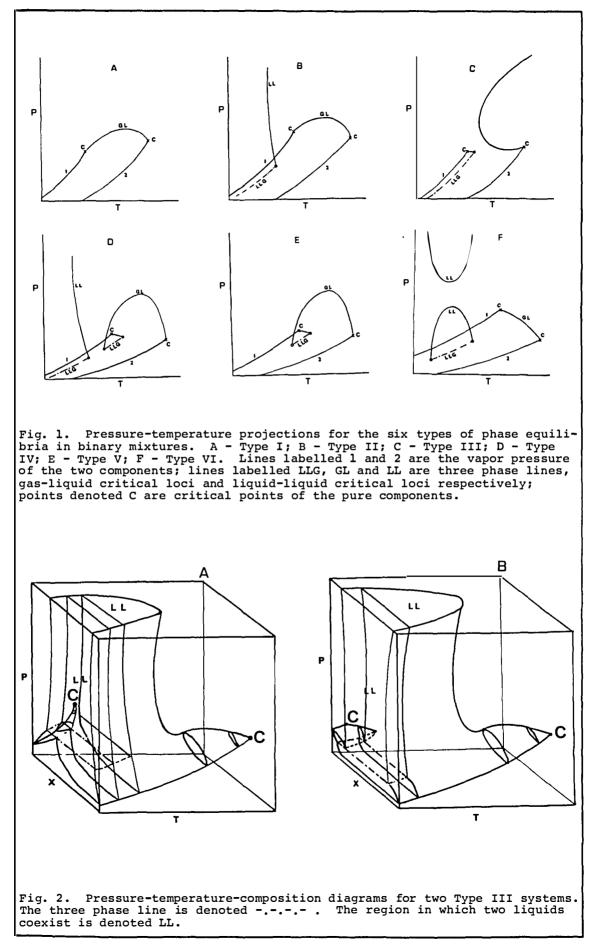
Type III. This phase diagram has two distinct critical lines, one starts at the critical point of the pure component with the higher critical temperature but never approaches the critical point of the other component moving rapidly to high pressures. The other critical line starts at the critical point of the component with the lower critical temperature and meets a three phase (liquid-liquid-gas) line in an UCEP. The three phase line may be between the vapor pressure curves of the two components (as shown in fig. 1C) or may be above the vapor pressure curves of both components. There are several subgroups in type III behavior depending on whether there is a heteroazeotrope or not and on the shape of the critical line starting at the critical point with the higher temperature.

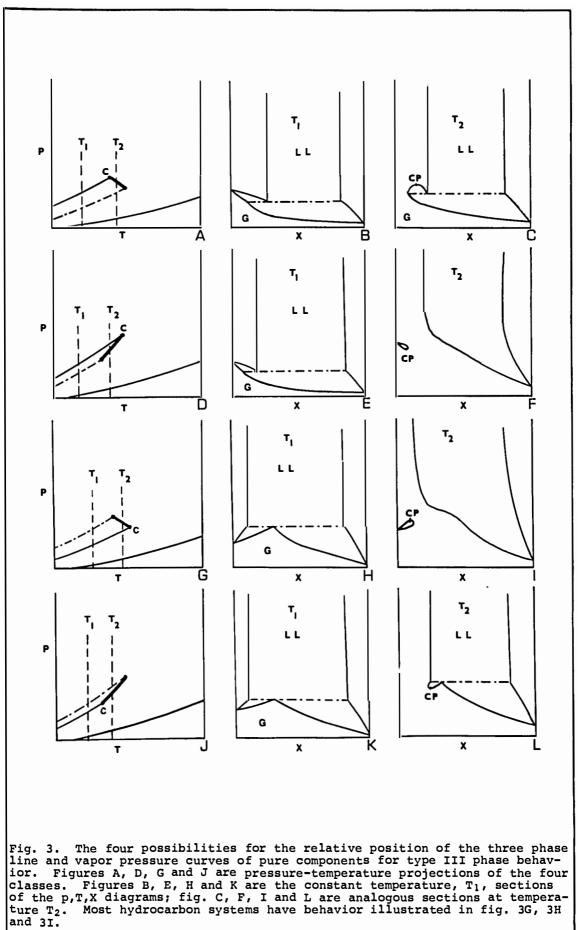
Type IV. This phase diagram has three distinct critical loci, one of which (the liquid-liquid critical line) starts at an UCEP on a three phase (liquid-liquid-gas) line and moves rapidly to higher pressures. The second line starts at the critical point of the component with the lower critical temperature and ends at an UCEP on a three phase line. The third line starts at the critical point of the other component and ends in a lower critical end point, LCEP, on the same three phase line as the second critical line.

Type V. This type is the same as type IV but without the liquidliquid critical line and the three phase line at lower temperatures.

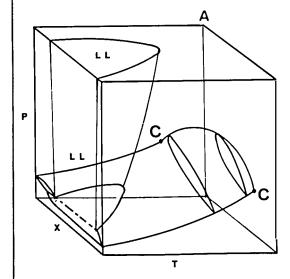
Type VI. This type of phase behavior is characterized by a continuous critical locus between the critical point of the two pure components. However, at lower temperatures there is a three phase line which is bounded above and below by critical end points. A liquid-liquid critical line joins these two critical end points. There are several known configurations of the line joining the ends of the three phase line. In the example illustrated (fig. 1F) the liquid-liquid critical line has two branches with a region of complete liquid miscibility between them.

Most hydrocarbon + water systems studied to date exhibit type III phase behavior. Typical pressure-temperature-composition diagrams for type III behavior are illustrated in fig. 2A and 2B. The most common type of phase behavior found in hydrocarbon water mixtures corresponds to fig. 2A. The behavior shown in fig. 2B has not yet been observed in hydrocarbon + water systems. From fig. 1 and 2 it can be seen that the three phase line on the pressure-temperature projection is derived from three lines on the pressure-temperature-composition diagram representing, the composition of gas, liquid 1 and liquid 2. **Phase Behavior**





There are many sub-types of type III behavior. Consider the portion of the phase diagram in the region of the upper critical end point and the critical point of the pure component with the lower critical temperature. There are four possibilities. The three phase line could be at higher or lower pressures than the vapor pressure curve of the pure component. Each of these two cases could have the upper critical end point at a higher (or lower) temperature than the critical point. These four possibilities are illustrated in fig. 3. The position of the vapor pressure of the second component can be above or below that of the first component. In the case of hydrocarbon + water systems the two pure component vapor pressure curves sometimes cross on the pressure-temperature projection (e.g. benzene + water). Most hydrocarbons + water systems exhibit the behavior illustrated in fig. 3G. Consider fig. 3G, the three phase line is at higher pressures than the vapor pressure of the pure component (1). At a temperature, T_1 , the pressure-composition diagram is shown in fig. 3H. It can be seen that depending on the pressure and overall composition it is possible to have one, two, or three phases present. At high pressures we have a fluid-fluid equilibrium which if T_1 is sufficiently low, it is reasonable to refer to as a liquid-liquid equilibrium. Although a line parallel to the composition axis at pressures between the three phase line and the vapor-pressure of component (1) cuts the boundary lines in four places, only two phases can be in equilibrium. The two phases in equilibrium will depend on the overall composition. At temperature T₂ a different situation exists in that at pressures above the critical line it is possible to have two phases present (fig. 3I). At pressures below the critical point it is possible to have two phases coexisting out of a possible four phases. Which are the two coexist-ing phases dependings on the overall composition. At some compositions only one phase will be present.



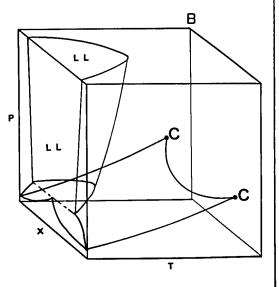


Fig. 4. Pressure, temperature, composition diagrams for two Type II systems. The three phase line is denoted -.-.-. The region in which two liquids coexist is denoted LL.

XX

Although most hydrocarbon + water systems studied to date exhibit type III phase behavior it is known that some hydrocarbons of greater molecular weight, such as biphenyl exhibit type II phase behavior 6. Figures 4A and 4B illustrate the pressure-temperature-composition diagram for two type II systems. It appears that most, if not all, hydrocarbon + water systems which exhibit type II behavior have a minimum in temperature for the gas-liquid critical curve which corresponds to the behavior illustrated in fig. 4B.

Some hydrocarbon + water systems have been observed to exhibit the phenomenon referred to as gas-gas immiscibility 6 . This phenomenon 5 occurs in type III phase behavior when the critical locus starting at the component with the highest critical temperature initially or eventually moves to high pressure at temperatures above the critical point of either component. If the critical locus always has a positive slope on the pressure-temperature projection the phenomenon is referred to as gas-gas immiscibility of the first kind (fig. 5A) whereas if the locus initially moves to lower temperatures, goes through a minimum and eventually moves to temperatures greater than the critical temperature of either component the mixture is said to exhibit gas-gas immiscibility of the second kind (fig. 5B). Gas-gas immiscibility of the second kind is exhibited by some hydrocarbon + water systems.

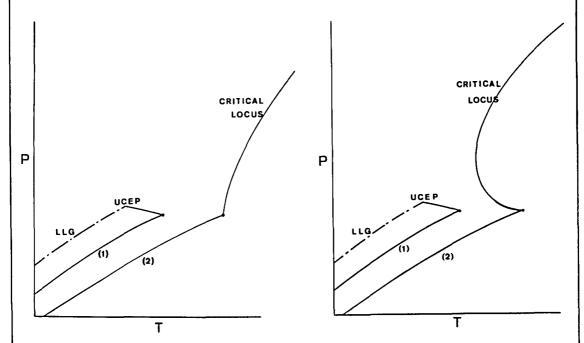


Fig. 5. Pressure, temperature projections for systems exhibiting gas-gas immiscibility. Figure 5A - immiscibility of the first kind. Figure 5B immiscibility of the second kind.

References.

- 1. Scott, R. L.; van Konynenburg, P. H.; Phil. Trans. Roy. Soc., London 1980, A298, 495.
- 2. Hicks, C. P.; Young, C. L.; Chem. Rev. 1975, 75, 119.
- 3. Gubbins, K. E.; Shing, K. S.; Streett, W. B.; J. Phys. Chem. 1983, 87, 4573.
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- 6. Brollos, K.; Peter, K.; Schneider, G. M.; Ber. Bunsenges. Phys. Chem. 1970, 74, 682. 7. De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N.; J. Chem.
- Thermodyn. <u>1982</u>, 14, 83. 8. Tsiklis, D. S.; Rott, L. A.; Russ. Chem. Rev. <u>1967</u>, 36, 351.

COMPONENTS:	EVALUATOR:
(1) Styrene; C ₈ H ₈ ; [100-42-5] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985

CRITICAL EVALUATION:

Quantitative solubility data for the styrene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies ofthe Styrene (1) - Water (2) System

L			
Reference	Т/К	Solubility	Method
Lane (ref 1)	298-324	mutual	various
Fordyce and Chapin (ref 2)	333	(l) in (2)	titration
Frilette and Hohenstein (ref 3)	298	(l) in (2)	unspecified
Andrews and Keefer (ref 4)	298	(l) in (2)	spectrophotometric
Banerjee <i>et al</i> . (ref 5)	298	(1) in (2)	HPLC

a Chemical analysis and cloud point measurements for (1) in (2). Karl Fischer and cloud point measurements for (2) in (1).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF STYRENE (1) IN WATER (2)

All the available data (ref 1-5) are listed in Table 2. At 298K the agreement among the independent measurements (ref 1,3-5) is reasonable but not sufficient to enable the average value to be Recommended.

At other temperatures, the value of Fordyce and Chapin (ref 2) at ~ 333K is very much higher than that of Lane (ref 1). Since the latter were obtained by two independent methods and, as already noted, are in fair agreement with other determinations at 298K, the datum of Fordyce and Chapin is rejected. In the absence of confirmatory studies the data at temperatures other than 298K should be regarded as very tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	July 1985.

CRITICAL EVALUATION: (continued)

TABLE 2.Tentative Values of the Solubilityof Styrene (1) in Water (2)

T/K	Solubility values		
	Reported values ^a	"Best" values	
	(g(l)/100g sln)	g(l)/l00g sln	10 ⁵ x ₁
283	0.29* (ref l)	0.029	5.0
293	0.030* (ref 1)	0.030	5.2
298	0.033* (ref 1), 0.022 (ref 3), 0.030 (ref 4), 0.016 (ref 5)	0.025 ± 0.006 ^b	4.3
303	0.034* (ref 1)	0.034	5.9
313	0.040* (ref 1)	0.040	6.9
323	0.046* (ref 1)	0.046	8.0
333	0.053* (ref 1), 0.95 (ref 2) ^c	0.053	9.2

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the author's two data sets, followed by averaging.

b Average (± σ_n) of all data; σ_n has no statistical significance. c At T = 333.5K, value rejected: see text.

2. THE SOLUBILITY OF WATER (2) IN STYRENE (1)

The solubility of water in styrene has been reported in only one study (ref 1) and thus no Critical Evaluation is possible. The interested user is referred to the relevant data sheet for the experimental solubility values.

REFERENCES

1. Lane, W.H. Ind. Eng. Chem. Anal. Ed. 1946, 18, 295-6.

2. Fordyce, R.G.; Chapin, E.C. J. Am. Chem. Soc. <u>1947</u>, 69, 581-3.

3. Frilette, V.J.; Hohenstein, W.P. J. Polym. Sci. <u>1948</u>, 3, 22-31.

4. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, ⁷², 5034-7.

 Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Env. Sci. Technol. <u>1980</u>, 14, 1227-9.

50_2	3
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Lane, W.H.
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. Anal. Ed. <u>1946</u> , 18, 295-6.
VARIABLES:	PREPARED BY:
Temperature: 7-65°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of a	styrene in water
<i>t/</i> °C g(l)100 g	$10^5 x_1$ (compiler)
(a) Formaldehyde - Sulfuric Acid Re	eagent Method
7 0.029	5.0
24 0.033	5.7
32 0.036	6.2
40 0.040	6.9
51 0.045	7.8
(b) Cloud Point Method	
15 0.025	4.3
25 0.031	5.3
44 0.040	6.9
49 0.045	7.8
56 0.050	8.6
65 0.058	10.0
AUXILIA	RY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
 (a) The solubility of (1) in (2) we determined by means of the formalde hyde-sulfuric acid reagent, ref (1) The value shown for 7°C is the mean of three determinations, and the value for 25°C is the mean of two determinations; all other data are single determinations only. (b) The cloud point exhibited by the system appeared to be very sharp, and the variable determination of the variable determination of	 samples; used as received. (2) not specified.
the samples passed from a state in which they were cloudy within 1°C.	ESTIMATED ERROR:
The cloud point data are averages of from two to eight separate determi- nations. Cloud points at 0.025 g(1 100 g solution were very faint.	of temp. (b) ± 0.5 °C (from two to
	REFERENCES:
	<pre>1. Morris, H.E.; Stiles, R.B.; Lane, W.H. Ind. Eng. Chem. Anal. Ed. 1946, 18, 294.</pre>

COMBONENTS		
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Lane, W.H.	
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. Anal. Ed. <u>1946</u> , 18, 295-6.	
VARIABLES:	PREPARED BY:	
Temperature: 6-51°C	A. Maczynski and Z. Maczynska	
-		
EXPERIMENTAL VALUES:		
Solubility of wa	ter in styrene	
t/°C g(2)/100 g	$10^3 x_2$ (compiler)	
(a) Karl Fischer Reagent Method		
6 0.032	1.8	
24 0.066	3.8	
31 0.084	4.8	
40 0.101	5.8	
51 0.123	7.1	
(b) Cloud Point Method		
14 0.040	2.3	
27 0.060	3.5	
34 0.080	4.6	
40 0.100	5.7	
45 0.120	6.9	
	· · · · · · · · · · · · · · · · · · ·	
	INFORMATION	
METHOD/APPARATUS/PROCEDURE:		
reinod/Arrakaius/rkoceduke:	SOURCE AND PURITY OF MATERIALS:	
(a) A large sample of (1) contain-	(1) source not specified; fresh	
ing a slight excess of (2) was shaken at a given temperature and	samples; used as received.	
then allowed to stand in a water bath at this temperature for 24 hr	(2) not specified.	
to ensure complete separation of		
the two phases before withdrawal of sample of the rich phase for titra-		
tion of the water present with the Karl Fischer reagent.		
(b) Duplicate determinations gave		
cloud points agreeing within 1°C, except in the case of 0.120 g(1)/	ESTIMATED ERROR:	
100 g solution where the agreement was within about 3°C. Cloud points	soly. (a) ± 1.5% (from two determi- nations)	
at 0.040 (1)/100 g solution were	temp. (b) \pm 1 to \pm 3°C.	
very faint. No more details were reported.	REFERENCES :	
-		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Fordyce, R.G.; Chapin, E.C.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1947</u> , 69, 581-3.
VARIABLES:	PREPARED BY:
One temperature: 60.3°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of styrene in water at 100 g(2).	60.3 C was reported to be 0.96 g(l)/
The corresponding mass percent and mol compiler are 0.95 g(l)/100 g sln and 1	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g por-	(1) Dow Chemical Co, N-100; redistilled.
tions of (2). The flasks were placed in a water-bath regulated to $60.3 \pm 0.02^{\circ}$ C. Component (1) was added a	(2) Not specified.
drop at a time to the water samples by means of a calibrated micro-pipet	
and the flasks agitated after each addition. The saturation point was	
taken at the first appearance of the turbidity and the amount of (1) was calculated from the number of drops	
added.	ESTIMATED ERROR:
	temp. ±0.02°C
	soly. ±0.05 g(1)/100 g sln
	REFERENCES :

5

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Frilette, V.J.; Hohenstein, W.P.
(2) Water; H ₂ O; [7732-18-5]	J. Polym. Sci. <u>1948</u> , 3, 22-31.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of styrene in water at 0.022 g(l)/100 g sln.	25°C was reported to be
The corresponding mole fraction, x_1 , compilers is 3.8 x 10^{-5} .	value calculated by the
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two different	(1) not specified.
ways. In the first method, conju- gated solutions were prepared by	(2) distilled.
shaking together excess (1) with (2) and allowing the layers to	
separate; the aqueous layer was then analyzed for (1). To avoid	
the possibility of contaminating the aqueous phase by small suspended droplets a second method was uti-	
lized; a cellophane sack, filled with (2) was completely submerged	ESTIMATED ERROR:
in a beaker containing (2); a layer of (1) was then floated on top of	Not specified.
(2) in the beaker. After 48 hr at 25°C, the sack was retrieved and	DEFEDENCIS.
the contents carefully removed and analyzed.	REFERENCES :
The method of analysis was not described.	
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of styrene in water at	25°C was reported to be 0.030 g(1)/
100 g sln.	
The corresponding mole fraction, x_1 , 5.19 x 10 ⁻⁵ .	calculated by the compilers is
1	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of (1) and (2) was rotated	SOURCE AND PURITY OF MATERIALS:
for twenty hours in a constant tem- perature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by	 (1) Eastman Kodak Co. white label; distilled shortly before use; l wt % of hydroquinone added as stabilizer before distilla- tion; b.p. 76 C (78 mm Hg). (2) Nat appendix distinct
shaking in a glass-stoppered Erlen- meyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spec- trophotometer.	(2) Not specified.
]	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Styrene; C ₈ H ₈ ; [100-42-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of styrene in water was sln. Assuming a solution density of per cent and mole fraction (x_1) solub are 0.0160 g(1)/100 g sln and 2.77 x	1.00 kg/L the corresponding mass ilities, calculated by the compiler,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experiments were performed in sealed	(1) Aldrich; purity not specified.
stainless steel centrifuge tubes. An excess of styrene was added to a tube containing distilled water, and the tube was sealed and allowed to equi- librate at 25 \pm 0.2°C with constant or intermittent shaking. Equilibra- tion was generally complete within 1 week. The mixture was then centri- fuged at 10,000 rpm for 60 min in a head preequilibrated to 25 \pm 0.3°C, following which aliguots of the solu-	(2) Distilled.
tion were removed for analysis by	ESTIMATED ERROR:
high-performance liquid chromato- graphy using a Waters M6000A instru-	Temperature: ±0.2°C
ment fitted with a C ₁₈ Bondapak column. The mobile phase was a mix-	Solubility: ±5.7% rel. (represen- ting one std. dev.)
ture of methanol/water or aceto- nitrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	REFERENCES:
	l

CRITICAL EVALUATION:

Quantitative solubility data for the o-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe o-Xylene (1) - Water (2) System

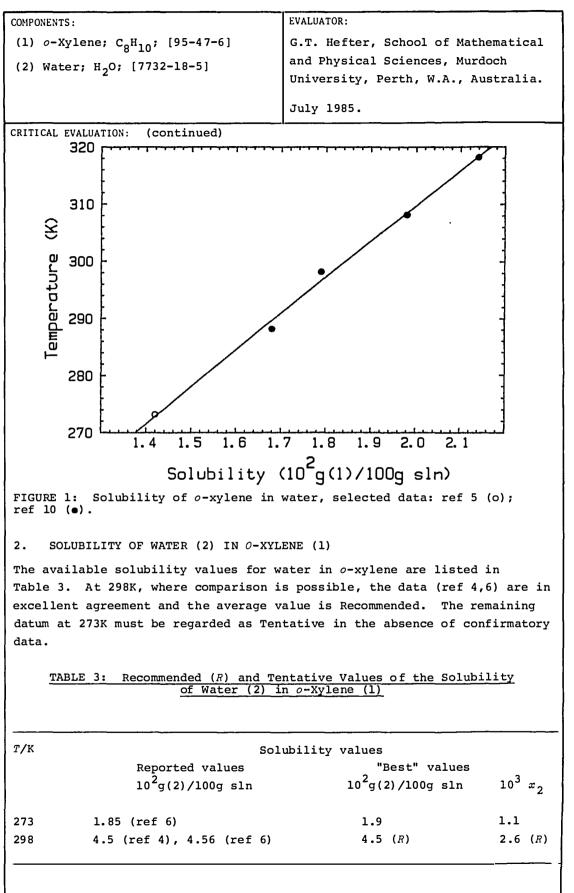
Reference	<i>т/</i> к	Solubility	Method
Andrews and Keefer (ref 1) Guseva and Parnov (ref 2) McAuliffe (ref 3)	298 385-524 298	<pre>(1) in (2) (1) in (2) (1) in (2)</pre>	spectrophotometric unspecified GLC
Hoegfeldt and Bolander (ref 4)		(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Price (ref 8)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(l) in (2)	GLC
Sanemasa <i>et al</i> . (ref 10)	299-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Alwani and Schneider (ref 5) have also reported data on a critical locus at high temperatures and pressures. For convenience further discussion of this system will be given in two parts.

1. SOLUBILITY OF O-XYLENE (1) IN WATER (2)

The high temperature, high pressure data of Guseva and Parnov (ref 2) and Alwani and Schneider (ref 5) have been obtained under quite different conditions and thus no Critical Evaluation of their data is possible. However, it may be noted that the data of Guseva and Parnov are frequently unreliable. The interested user is referred to the relevant Data Sheets for experimental values.

At atmospheric pressure all the available data are listed in Table 2 except for the value of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) and has therefore been excluded from consideration.



(continued next page)

COMPONENTS: (1) <i>o</i> -Xylene; C ₈ H ₁₀ ; [95-47-6] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	July 1985

CRITICAL EVALUATION: (continued)

At 298K, the data of McAuliffe (ref 3), Sutton and Calder (ref 7), Price (ref 8) and Sanemasa *et al.* (ref 10) are in excellent agreement and their average is Recommended. The values of Andrews and Keefer (ref 1) and Polak and Lu (ref 6) are markedly higher ($>3\sigma_n$) and are rejected.

At other temperatures only the data of Sanemasa $et \ all$. (ref 10) are available except for the 273K datum of Polak and Ly (ref 6). These data are therefore regarded as Tentative.

Selected data are plotted in Figure 1.

 TABLE 2:
 Recommended (R) and Tentative Solubility Values of

 o-Xylene
 (1) in Water

T/K	Solubility Reported values 10 ² g(1)/100g sln	y values "Best" values 10 ² g(1)/100g sln	
273	1.42 (ref 5)	1.4	2.4
288	1.68 (ref 10)	1.7	2.9
298	1.75 (ref 3), 1.705 (ref 7), 1.67 (ref 8), 1.79 (ref 10)	1.73 ± 0.05 (R)	2.93 (R)
308	1.98 (ref 10)	2.0	3.4
318	2.14 (ref 10)	2.1	3.6

a Obtained by averaging where appropriate; $\sigma_{\mathbf{n}}$ has no statistical significance.

(continued next page)

COMPONENTS: EVALUATOR: (1) *o*-Xylene; C₈H₁₀; [95-47-6] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. July 1985 (continued) CRITICAL EVALUATION: REFERENCES 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-7. Guseva, A.N.; Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9. 2. McAuliffe, C. Nature 1963, 200, 1092-3; J. Phys. Chem. 1966, 70, з. 1267-72. 4. Hoegfeldt, E.; Bolander, B. Ark. Kemi 1964, 21, 161-86. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. 1969, 73, 294-301. 5. Polak, J.; Lu, B. C-Y. Can. J. Chem. 1973, 51, 4018-23. 6. 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44; see also Ph.D. Dissertation, <u>1973</u>, Univ. California, Riverside, CA, U.S.A., 8. quoted in ref 10. 1978, 34, 413-7. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 9. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62. 10. ACKNOWLEDGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Andrews, L.J.; Keefer, R.M.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of o-Xylene in water at	-25° C was reported to be	
0.0204 g(1)/100 g sln.	25 C was reported to be	
The corresponding mole fraction, x_1 , calculated by the compilers is 3.46 x 10 ⁻⁵ .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	(1) Eastman Kodak Co. best grade; fractionally distilled; b.p.	
perature bath at 25°C. A sample	range 144.3-144.5°C.	
(5-20 mL) of the aqueous phase was withdrawn and extracted with a	(2) Not specified.	
measured volume of hexane (10-50 mL) by shaking in a glass-stoppered		
Erlenmeyer flask. Next, the absorb-		
ance of the hexane phase wa's meas- ured against a hexane blank on the		
Beckman spectrophotometer.		
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS :		ORIGINAL MEASUREMENTS:
(1) o-Xylene; (C ₈ H ₁₀ ; [95-47-6]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ 0;	· -·	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.
VARIABLES:		PREPARED BY:
Temperature: 1	139-251°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES	:	
	Solubility of o-	vulene in water
	Solubility of 0	Aylene in water
	t/°C g(l)/100 g	$\frac{10^4 x_1 \text{ (compiler)}}{10^4 x_1 \text{ (compiler)}}$
	139 0.047 162 0.093	0.80
	207 0.407	1.58 6.93
	251 0.960	16.42
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PR		SOURCE AND PURITY OF MATERIALS:
The measurement		(1) source not specified;
sealed glass tu	ubes. No details	$n_{\rm D}^{20}$ 1.5054.
were reported i	th the paper.	- ,
		(2) doubly distilled.
		ESTIMATED ERROR:
		not specified.
		REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1963</u> , 200, 1092-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-Xylene in water at	25°C was reported to be
0.0175 g(1)/100 g sln.	
The corresponding mole fraction, x_1 , o	calculated by the compilers is
2.97×10^{-5} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in (2) was prepared by either shaking vigor-	(1) Phillips Petroleum Co.; 99+%; used as received.
ously on a reciprocal shaker or stir-	
ring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample	(2) Distilled.
of the hydrocarbon-saturated water was injected directly into a gas	
liquid chromatograph.	
	ESTIMATED ERROR:
	Temp. ±1.5°C
	Soly. 0.0008 (std. dev. of mean)
	REFERENCES:
,	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) $2-3$ (1) (Hoegfeldt, E.; Bolander, B.
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	-
(2) Water; H ₂ O; [7732-18-5]	Ark. Kemi, <u>1964</u> , 21, 161-86.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
	A. Muczynski und z. Muczynsku
EXPERIMENTAL VALUES:	
The solubility of water in o-Xylene wa	as reported to be 0.022 mol(2) L sln.
The corresponding mass percent and mo	I fraction, x_2 , calculated by the
compilers are 0.045 g(2)/100 g sln and	1 0.0026.
The assumption that 1.00 L sln = 876 o	g sln was used in the calculation.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The water determination was carried	(1) Fluka; 0.7% of (m-p) xylene,
out according to Johansson's modifi- cation of the Karl Fischer titration	0.07% of ethylbenzene; purity 99.0%; used as received.
in ref 1, 2.	99.0%; used as received.
	ESTIMATED ERROR:
	Temp, ±0,3 C
	Soly. ±0.002 mol(2) L ⁻¹ sln (type of error not specified)
	REFERENCES:
	1. Hardy, C.J.; Greenfield, B.F.;
	Scargill, D. J. Chem. Soc. 1961, 90.
	2. Johansson, A. Sv. Papperstidn. 1947, 11B, 124.
	<u>1347,</u> 110, 124.

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COMPONENTS:		OR	IGINAL MEASUREMEN	NTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]		P	Polak, J.; Lu, B.CY.	
(2) Water;	H ₂ O; [7732-18-5]	С	an. J. Chem.	<u>1973</u> , <i>51</i> , 4018-23.
VARIABLES:				
			EPARED BY:	
Temperatur	e: 0-25°C	A	. Maczyński ar	nd Z. Maczynska
EXPERIMENTAL	VALUES:			
	Solubility of	of o-xyl	ene in water	-
t/°C	mg(1)/kg(2)	g(l)/ (co	100 g sln mpiler)	$10^{5} x_1$ (compiler)
0(a)	142(c)		0.0142	2.41
25 (b)	213(c)		0.0213	3.61
	Solubility o	of water	in o-xylene	
t/°C	mg(2)/kg(1)		100 g sln mpiler)	$10^{3}x_{2}$ (compiler)
0(a)	185 (d)		0.0185	1.09
25 (b)	456 (e)		0.0456	2.68
		LIARY INF	ORMATION	
METHOD/APPARA	IUS/PROCEDURE:	SO	URCE AND PURITY C	OF MATERIALS:
with (2) w Hypo-vial teflon coa placed in water bath magnetical the bath with	ly for 24 hr and left or 3 days or was kept	a (red in		ganics, pure grade baken three times led water.
for analys	ithout stirring for 7 re samples were taken is.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-xylene in water a	at 25°C was reported to be
170.5 mg(1)/kg(2). The corresponding	g mass percent and mole fraction,
x_1 , calculated by the compilers are (0.01705 g(l)/100 g sln and
2.892×10^{-5} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR: temp. ± 0.1°C
	soly. 2.5 mg(1)/kg(2) (the standard deviation of the
	mean for six replicates)
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [97-47-6]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

The solubility of o-xylene in water at 25°C and at system pressure was reported to be 167.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0167 g(1)/100 g sln and 2.83 x 10⁻⁵.

AUXILIARY	INFORMATION
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The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

- Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
- (2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 4.0 mg(1)/kg(2)

REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [97-47-6]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of o-xylene in water a	at 25°C was reported
to be 167.0 mg(1)/kg(2).	
The corresponding mass percent and me	ole fraction, x_1 , calculated
by compiler are 0.0167 g(1)/100 g sl	n and 2.83 x 10^{-5} .
Editor's Note: Based on the results systems, uncertainity exists about w	for this and other hydrocarbon-water
independent of that of Price for the	
-	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in	(1) not specified.
(2) were prepared in two ways. First, 200 µL of (1) was injected	(2) not specified.
into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	
and (2) as above was thermostated at 70°C and then cooled to 25°C. The	-
time required to obtain equilibrium was three weeks. The solubility of	-
(1) in (2) was measured by glc. A	
Perkin-Elmer model F-ll gas chromat- ograph equipped with a 100-150 mesh	
Porasil column (70°C) and a flame ionization detector was used. Sat-	ESTIMATED ERROR:
urated solutions of heptane in (2) were used as standard solutions.	soly. 4.2 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES:
	I

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38_15			
COMPONENTS:	•	ORIGINAL MEASUREMENTS:	
(1) <i>o</i> -Xylene:	C ₈ H ₁₀ ; [97-47-6]	Sanemasa, I.; Araki	. M.:
(2) Water; H ₂ O		Deguchi, T.; Nagai,	
(-,		Bull. Chem. Soc. Jpn.	
ARIABLES:		PREPARED BY:	
Cemperature: 1	5-45°C	G.T. Hefter	
XPERIMENTAL VALU	ES:		
	The solubility of	o-xylene in water	
t/°C	$10^3 \text{ mol}(1)/\text{dm}^3 \text{ sln}$	q(1)/100 q sln	10 ⁵ x ₁
••• •	(_ ,	(compiler) ^a	(compiler) ^a
		(00	
15	1.58 ± 0.11	0.0168	2.85
25	1.68 ± 0.06	0.0179	3.04
35	1.85 ± 0.02	0.0198	3.35
45	2.00 ± 0.02	0.0214	3.64
	AUXILIARY	INFORMATION	
ETHOD/APPARATUS/	PROCEDURE:	SOURCE AND PURITY OF MAT	TERIALS;
earlier design lescribed in de LOO-200 cm ³ of Liquid (1) were	is similar to an (ref 2) and is etail in the paper. (2) and 10-20 cm ³ of e placed in separate thermostatted flasks.	Pure Chemical purity 98.0%, further purifi	
fter thermal of ished a recirco as used to var o transport the ontaining (2)	equilibrium was estab- culating stream of air porize liquid (1) and ne vapor to the flask . Five 10 cm ³ aliquots	given.	
	into separatory concentration of (1) in	ESTIMATED ERROR:	
2) was then dents of the chloroform	etermined by extraction n followed by UV- try. Standards for the try were prepared by	<pre>soly. see table, ty specified. temp. ± 0.1°C.</pre>	pe of error not
	re liquid solutes.	REFERENCES :	
		1. Kell, G.S. J. Chem. Eng. Data	1975, <i>20.</i> 97.
		 Sanemasa, I.; A Deguchi, Y.; Na 	 raki, M.;
		Chem. Lett. 1981	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref l)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of o-xylene in artifi	
129.6 mg(1)/kg sln. The correspondi	_
x_1 calculated by the compiler are 0.	
assuming the artificial seawater com	position of ref 1.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.
chiomatography.	
	1
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 1.8 (std. dev.)
	REFERENCES: 1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.

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COMPONENTS:	EVALUATOR:
(2) Water: H_O: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986

CRITICAL EVALUATION:

Quantitative solubility data for the m-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe m-Xylene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-313	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	344-544	(1) in (2)	synthetic
Guseva and Parnov (ref 4)	400-512	(1) in (2)	${\tt unspecified}^a$
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Englin <i>et al</i> . (ref 6)	283-303	(2) in (1)	analytical
Polak and Lu (ref 7)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 8)	298	(1) in (2)	GLC
Chernoglazova and Simulin (ref 9)	293-343	mutual	synthetic, GLC
Price (ref 10)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 11)	298	(l) in (2)	GLC
Sanemasa <i>et al</i> . (ref 12)	288-318	(1) in (2)	spectrophotometric

a The synthetic method was probably used.

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

1. SOLUBILITY OF M-XYLENE (1) IN WATER (2)

All the available data for the solubility of m-xylene in water at low temperatures ($T \leq 343$ K) are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 11) which does not appear to be independent of that of Price (ref 10) and has therefore been excluded from consideration.

The data are in general in reasonable agreement although with a few exceptions the agreement is insufficient for the average values to be Recommended. Selected data from Table 2 are plotted in Figure 1.

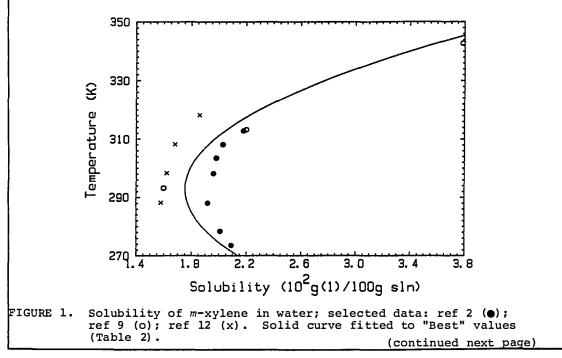
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COMPONENTS :	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986

TABLE 2: Recommended (R) and Tentative Values of the Solubilityof m-Xylene (1) in Water (2)

<i>т/</i> к	Solubili	ty values	
	Reported values ^a	"Best" values "Best" values 10 ² g(1)/100g sln	$(\pm \sigma_n)^b$
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	10 ⁵ x ₁
273	2.10* (ref 2), 1.96 (ref 7)	2.03 ± 0.07 (R)	3.44 (R)
283	1.97* (ref 2)	2.0	3.4
293	1.95* (ref 2), 1.6 (ref 9) 1.60* (ref 12)	1.7 ± 0.2	2.9
298	1.73 (ref 1), 1.96 (ref 2), 1.62 (ref 7), 1.46 (ref 8), 1.7* (ref 9), 1.34 (ref 10), 1.62 (ref 12)	1.6 ± 0.2	2.7
303	1.98* (ref 2), 1.8* (ref 9), 1.65* (ref 12)	1.8 ± 0.1	3.1
313	2.19* (ref 2), 2.2 (ref 9)	2.20 (R)	3.73 (R)
323	2.6* (ref 9), 2.0* (ref 12)	2.3 ± 0.3	3.9
333	3.2* (ref 9)	3.2	5.4
343	3.5* (ref 3)	3.5	5.9

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.
 b Obtained by averaging where appropriate; σ_n has no statistical significance.



COMPONENTS:	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

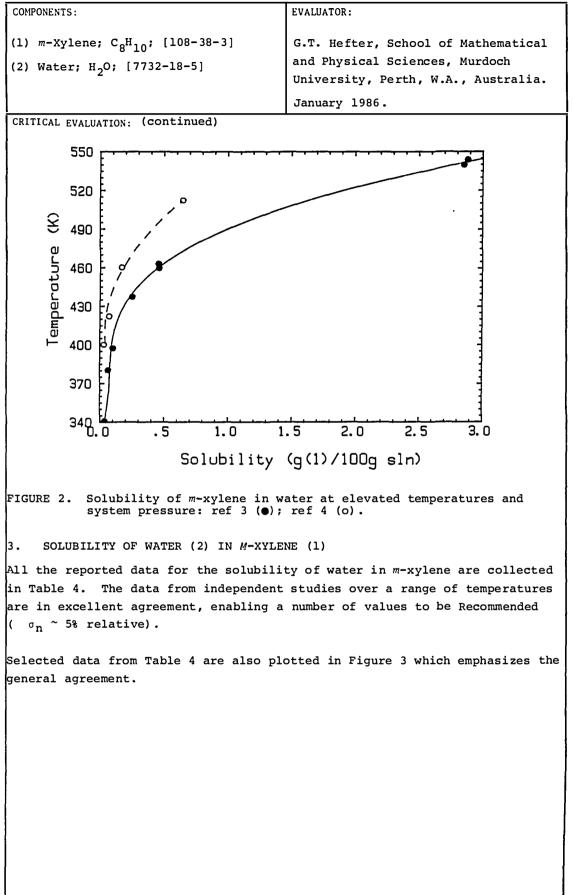
Table 3 summarizes thermodynamic functions calculated by application of the van't Hoff equation to the solubility data obtained over various temperature ranges. At low temperatures (T < 343K) the values of ΔH_{sln} and $\Delta C_{p,sln}$ from the data of Bohon and Claussen (ref 2) and Sanemasa *et al.* (ref 12) are in good agreement (Table 3) and are close to calorimetric values reported for similar systems (*e.g.* benzene in water, ref 13). However, the ΔH_{sln} derived from the data of Chernoglazova and Simulin (ref 9) is much too positive.

TABLE 3: Thermoydnamic Function for the Dissolution of m-Xylene in Water Derived from Solubility Data

Reference	^{AH} sln kJ mol ⁻¹	^{ΔC} p,sln J K ⁻¹ mol-1
Bohon and Claussen (ref 2)	2.8	386
Pryor and Jentoft (ref 3)	8.6	200
Guseva and Parnov (ref 4)	36.7	55
Chernoglazova and Simulin (ref 9)	11.4	167
Sanemasa (ref 12)	2.6	317
"Best" values (Table 2)	2.9	516

2. SOLUBILITY OF M-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for *m*-xylene in water at elevated temperatures (*ca*. 340-550K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 14). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of comfirmatory studies it is difficult to know which values are more reasonable. However, it may be noted that the thermodynamic functions derived from the data of Pryor and Jentoft are more reasonable than those obtained from Guseva and Parnov's work (Table 3). The interested user is referred to the relevant Data Sheets for the experimental values.



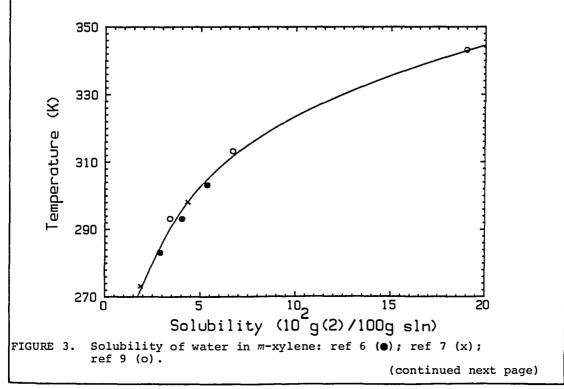
COMPONENTS:	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

TABLE 4: Recommended (R) and Tentative Values of the Solubilityof Water (2) in m-Xylene (1)

T/K	Solubil	ity values	
1	Reported values ^a	"Best" value	$s (t \sigma_n)^b$
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	10 ³ <i>x</i> 2
273	1.88 (ref 7)	1.9	1.1
283	2.89 (ref 6), 2.8* (ref 7)	2.9 ± 0.1 (R)	1.7(R)
293	4.02 (ref 6), 3.7* (ref 7), 3.4 (ref 9)	3.7 ± 0.3 (R)	2.2 (<i>R</i>)
298	4.4 (ref 5), 4.7* (ref 6), 4.32 (ref 7), 4.0 (ref 9)	4.4 ± 0.3 (R)	2.6 (<i>R</i>)
303	5.36 (ref 6), 4.8 (ref 9)	5.1 ± 0.3 (R)	3.0(<i>R</i>)
313	6.7 (ref 9)	6.7	6.7
323	10* (ref 9)	10	5.9
333	14* (ref 9)	14	8.3
343	19* (ref 9)	19	11

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

b Calculated by averaging where appropriate; σ_{n} has no statistical significance.



COMPONENTS:	EVALUATOR:
<pre>(1) m-Xylene; C₈H₁₀; [108-38-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

Application of the van't Hoff equation to the data of Englin *et al.* (ref 6) and Chernoglazova and Simulin (ref 9) gives values for ΔH_{sln} of 21.3 and 24.9 kJ mol⁻¹ and for $\Delta C_{p,sln}$ of -152 and 208 J K⁻¹ mol⁻¹ respectively. Comparison with related systems (*e.g.* water in benzene) suggests the data of Chernoglazova and Simulin (ref 9) may be more reliable.

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- 8. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
- Chernoglazova, F.S.; Simulin, Yu.N. Zh. Fiz. Khim. <u>1976</u>, 50, 809; Deposited doc. 1976, VINITI 3528-75.
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ACKNOWLEDGEMENT

The evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of m-Xylene in water a	t 25°C was reported to be
0.0173 g(l)/100 g sln. (value updat	ed from original paper)
The corresponding pole function of	algulated by the compilers is
The corresponding mole fraction, $x1$, 2.93 x 10-5.	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	(1) Eastman Kodak Co. best grade; fractionally distilled;
perature bath at 25°C. A sample (5-20 mL) of the aqueous phase was	b.p. 139.5°C.
withdrawn and extracted with a mea- sured volume of hexane (10-50 mL)	(2) Not specified.
by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb-	
ance of the hexane phase was mea- sured against a hexane blank on the	
Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

(1) m-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O ; [7732-18-5] VARIABLES: Temperature: 0.4-39.6°C EXPERIMENTAL VALUES: t/°C $(comp: 0.4]{0.4}$ 0.02 0.02 0.02 0.02 0.02	$\log \sin^{\alpha}$ $\log^{5} x_{1}$	
(2) Water; H_2O ; [7732-18-5] VARIABLES: Temperature: 0.4-39.6°C EXPERIMENTAL VALUES: t/°C (comp) 0.4 5.2 0.02	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8. PREPARED BY: G.T. Hefter xylene in water $\log \sin^a \qquad \log^5 x_1$	
VARIABLES: Temperature: 0.4-39.6°C EXPERIMENTAL VALUES: t/°C (comp:) 0.4 5.2 0.02	PREPARED BY: G.T. Hefter xylene in water 0g sln^a 10^5x_1	
Temperature: $0.4-39.6^{\circ}C$ EXPERIMENTAL VALUES: $t/^{\circ}C$ $g(1)/100$ (comp: 0.4 0.02 5.2 0.02	G.T. Hefter xylene in water $\log \sin^a \qquad \log^5 x_1$	
Temperature: $0.4-39.6^{\circ}C$ EXPERIMENTAL VALUES: $t/^{\circ}C$ $g(1)/100$ (comp: 0.4 0.02 5.2 0.02	G.T. Hefter xylene in water $\log \sin^a \qquad \log^5 x_1$	
EXPERIMENTAL VALUES: 501ubility of m-5 t/°C g(1)/100 (comp: 0.4 0.02 5.2 0.02	xylene in water 0g sln ^a $10^5 x_1$	
Solubility of m	$\log \sin^a \qquad 10^5 x_1$	
Solubility of m	$\log \sin^a \qquad 10^5 x_1$	
0.4 0.02 5.2 0.02		
5.2 0.02		
	209 3.54 201 3.41	
14.9 0.01		
	192 3.25 196 3.33	
	196 ^b 3.33 ^b	
25.6 0.0		
30.3 0.03		
34.9 0.02		
39.6 0.02	218 3.69	
b Given in the original paper as 0.196g(l)/L sln.		
AUXILIARY I	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette	<pre>(1) Oronite Chemical Co. was sulphonated, hydrolysed, steam distilled, washed, dried by passing through silica gel and finally distilled. Purity was judged by refractometry (no value given). (2) Air-free conductivity water (no details given). (2) Air-free conductivity water (no details given). ESTIMATED ERROR: Temp. ± 0.02°C Soly. ± 0.5% relative REFERENCES:</pre>	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Pryor, W.A.; Jentoft, R.E.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1961</u> , 6, 36-7.
VARIABLES:	PREPARED BY:
Temperature: 67.7-270.6°C	A. Maczynski and Z. Maczynska

	t/°C		2	
Cloud point appears	Cloud point disappears	Midpoint	<u> </u>	g(l)/100 g sln (compiler)
64.4	71.1	67.7	0.0590	0.0348
105.6	109.0	107.3	0.1127	0.0664
122.7	125.6	124.2	0.1749	0.1031
162.7	165.6	164.2	0.4265	0.2509
185.6	187.3	186.4	0.7825	0.4595
187.8	190.0	189.9	0.7762	0.4559
264.4	268.9	266.6	4.956	2.852
-	270.6	270.6	5.00	2.88

Solubility of m-xylene in water

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dis- solved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud dis- appeared. The cycle was repeated three to four times until reliable appearance and disappearance temper- atures for the cloud were recorded.	 source not specified; 99.8% by freezing point; main impurities are isomeric xylenes; used as received. not specified. 	
	ESTIMATED ERROR: not specified.	
	REFERENCES:	

COMPONENTS:	OPICINAL MEASUDEMENTS.	
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I.	
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76 - 9.	
VARIABLES:	PREPARED BY:	
Temperature: 127-239°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:	a	
Solubility of m-:	xylene in water	
t/°C g(1)/100 g	$\frac{10^4 x_1}{(\text{compiler})}$	
127 0.031 149 0.072	0.53	
187 0.168	1.22 2.85	
239 0.648	11.06	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n _D ²⁰ 1.4974.	
	(2) doubly distilled.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Hoegfeldt, E.; Bolander, B.
(2) Water; H ₂ O; [7732-18-5]	Ark. Kemi, <u>1964</u> , 21, 161-86.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of water in m-Xylene w	as reported to be 0.021 mol (2) L^{-1}
sln.	
The corresponding mass percent and mo	
compilers are 0.044 g(2)/100 g sln and	a 0.0026.
The assumption that 1.00 L sln = 860 of	s eln was used in the calculation
The assumption that 1.00 L sin = 800 (g sin was used in the calculation.
AUXILIARY	INFORMATION
	SOURCE AND PURITY OF MATERIALS:
The water determination was carried	(1) Fluka; 0.3% of ethylbenzene,
out according to Johansson's modifi- cation of the Karl Fischer titration	0.03% of o-Xylene; purity 99.6%; used as received.
in ref 1, 2.	(2) Not specified.
	(2) Not specified.
	ESTIMATED ERROR: Temp. ±0.03°C
	Soly. $\pm 0.001 \text{ mol}(2) \text{ L}^{-1} \text{ sln}$ (type
	of error not specified)
	REFERENCES:
	<pre>1. Hardy, C.J.; Greenfield, B.F.; Scargill, D.</pre>
	J. Chem. Soc. <u>1961</u> , 90.
	2. Johansson, A. Sv. Papperstidn. 1947, 11B, 124.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(l) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of W <u>t/°C</u> <u>g(2)/100 g sln</u> 10 0.0289 20 0.0402 30 0.0536	ater in m-Xylene $\frac{10^3 x_2 \text{ (compiler)}}{1.70}$ $\frac{2.37}{3.15}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hy- dride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<pre>(1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.</pre>
	REFERENCES:

38_24					3
COMPONENTS :			ORIGINAL MEASUREM	ENTS:	
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]		Polak, J.; Lu, B.CY.			
(2) Water;	H ₂ O; [7732-18-5]		Can. J. Chem.	<u>1973</u> , <i>51</i> , 4018~23.	
VARIABLES:			PREPARED BY:		
Temperatur	ce: 0-25°C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL	VALUES:	 	<u> </u>		
	Solubility	of m-x	ylene in water		
t/°C	mg(1)/kg(2)	g(1 ()/100 g sln compiler)	$10^{5}x_{1}$ (compiler)	
0(a)	196(c)		0.0196	3.32	
25 (b)	162(c)		0.0162	2.75	
	Solubility	of wat	er in m-xylene		
<i>t/</i> °C	mg(2)/kg(1))/100 g sln compiler)	$10^{3}x_{2}$ (compiler)	
0(a)	188(d)		0.0188	1.11	
25 (b)	432(e)		0.0432	2.54	
^{a-e} See "Estimated Error"					
AUXILIARY INFORMATION					
METHOD/APPARAT	rus/Procedu Re:	5	SOURCE AND PURITY	OF MATERIALS:	j
with (2) w Hypo-vial teflon coa placed in water bath magnetical the bath for the bath w	ly for 24 hr and lef- or 3 days or was kep ithout stirring for re samples were takes	mL h a d re irred t in t in 7		reagent (99+%); ee times with	
The solubi organic la Karl Fisch solubility	lity of water in the yer was determined by er titration and the of hydrocarbon in the r was determined by a	y he gas	soly. (c) \pm 1.	02°C, (b) ± 0.01°C 7%, (d) ± 4.7%, 1% (from two or three ations)	2

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of m-xylene in water a	t 25°C upg reported to be
146.0 mg(1)/kg(2). The corresponding	
x_1 , calculated by the compilers are 0 2.48 x 10 ⁻⁵ .	.01400 g(1)/100 g Sin and
2.48 x 10 ⁻ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma-	(1) Aldrich Chemical Co. or Matheson Coleman and Bell
tography.	99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. $\pm 0.1^{\circ}C$
	soly. 1.6 mg(1)/kg(2) (the standard deviation of the
	<u>mean for six replicates)</u> REFERENCES:

38_26

30_20	57	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Chernoglazova, F.S.; Simulin, Yu.N. Zh. Fiz. Khim. <u>1976</u> , 50, 809.	
(2) water; $n_20; [7732-10-5]$	Deposited doc. <u>1976</u> , VINITI 3528-75.	
VARIABLES:	PREPARED BY:	
Temperature: 20-70°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of m	-Xylene in Water	
<u>t/°C</u> <u>g(1)/100</u>	g sln 10 ⁵ x ₁ (compiler)	
20 0.016 40 0.022		
70 0.038		
Solubility of Water in m-Xylene		
<u>t/°C</u> g(2)/100	g sln 10 ³ x ₂ (compiler)	
20 0.034 40 0.067		
70 0.190	11.1	
	-	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility of (1) in (2) was determined by the synthetic method of	<pre>(1) Source not specified; 99.9 purity by glc.</pre>	
Fuhner, ref 1. Glass tubes filled with 50-100 mL of (2) were frozen and then (1) was micropipetted. Next,	(2) Distilled.	
the tubes were sealed and thermo- statted for 6 hrs at 70°C and 72 hrs		
at 20°C. The solubility was followed visually. The samples were incre-		
mented at regular steps 0.005 g $(1)/100$ g (2) . The mean value from 5-6		
determinations was adopted.	ESTIMATED ERROR:	
The solubility of (2) in (1) was determined by gas chromatography. The LKhM-7a instrument equipped with	Not specified.	
a katharometer was employed.	REFERENCES :	
	1. Fuhner, H.; Chem. Ber. <u>1924</u> , 57, 514.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

The solubility of m-xylene in water at 25°C and at system pressure was reported to be 134.0 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0134 g(l)/100 g sln and 2.27 x 10⁻⁵.

AUXILIARY INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<pre>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 2.0 mg(1)/kg(2) REFERENCES:</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Krzyzanowska, T.; Szeliga, J.	
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:	-	
The solubility of m-xylene in water at 25°C was reported		
to be 134.0 mg(1)/kg(2).		

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 0.0134 g(1)/100 g sln and 2.27 x 10^{-5} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat-	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR: soly. 3.4 mg(1)/kg(2) (standard</pre>
urated solutions of heptane in (2) were used as standard solutions.	deviation from 7-9 determinations).
	REFERENCES:

•

40	. 38_29
COMPONENTS :	ORIGINAL MEASUREMENTS:
(l) m-Xylene; C ₈ H ₁₀ ; [108-38-3] (2) Water; H ₂ O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.
VARIABLES:	PREPARED BY:
Temperature: 15-45°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of	<i>m-</i> xylene in water
t/°C 10 ³ mol(1)/dm ³ sln	$\begin{array}{c} g(1)/100 \ g \ sln \\ (compiler)^{a} \end{array} \begin{array}{c} 10^{5} \ x_{1} \\ (compiler)^{a} \end{array}$
15 1.49 ± 0.04	0.0158 2.68
25 1.52 ± 0.06	0.0162 2.75
35 1.57 ± 0.10	0.0168 2.85
45 1.73 ± 0.08	0.0186 3.15
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by	 Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification. Redistilled; no further details given.
	ESTIMATED ERROR: soly. see table, type of error not specified. temp. ± 0.1°C.
weight from pure liquid solutes.	REFERENCES:
	1. Kell, G.S. J. Chem. Eng. Data <u>1975</u> , 20 , 97.
	 Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. <u>1981</u>, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C ₈ H ₁₀ ; [108-38-3]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	I
The solubility of m-xylene in artifi	cial seawater is reported to be
106.0 mg(1)/kg sln. The correspondi	ng mass percent and mole fraction,
x_1 calculated by the compiler are 0.	01060 g(1)/100 g sln and 1.85 x 10^{-5}
assuming the artificial seawater com	
	-
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The	
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.6 (std. dev.)
	REFERENCES:
	<pre>1. Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.</pre>

CRITICAL EVALUATION:

Quantitative solubility data for the p-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-316	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	316-577	(l) in (2)	synthetic
Guseva and Parnov (ref 4)	414-531	(1) in (2)	unspecified
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(l) in (2)	GLC
Kirchnerova and Cave (ref 8)	298	(2) in (1)	Karl Fischer
Price (ref 9)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 10)	298	(l) in (2)	GLC
Sanemasa <i>et al</i> . (ref ll)	288-318	(l) in (2)	spectrophotometric

TABLE 1: Quantitative Solubility Studies of thep-Xylene (1) - Water (2) System

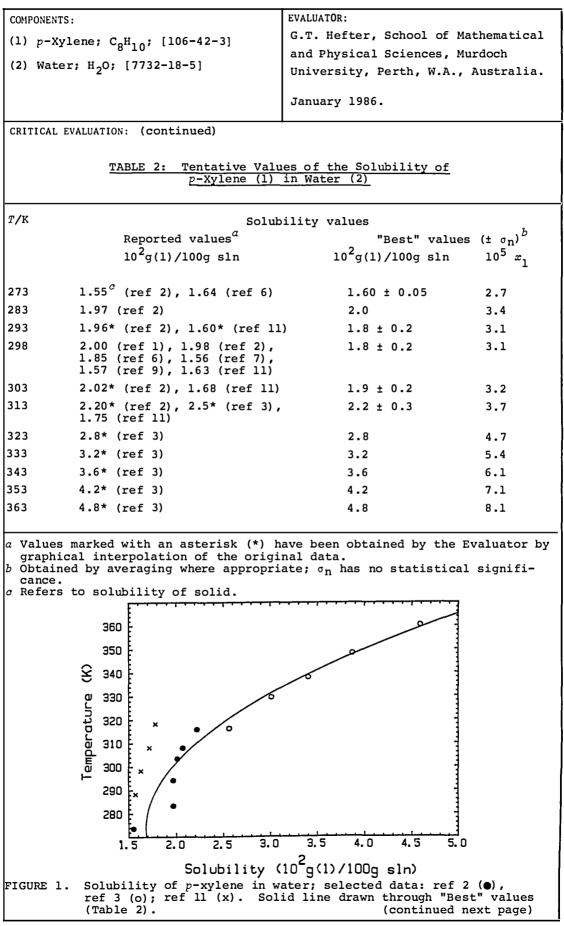
January 1986.

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

SOLUBILITY OF p-XYLENE (1) IN WATER (2)

All the available data on the solubility of p-xylene in water are summarized in Table 2 with the exception of the high temperature data of Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4) which are discussed in the next section. The 298K datum of Krzyzanowska and Szeliga (ref 10) has also been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 9).

The various data for *p*-xylene in water (Table 2) are in only fair agreement and none of the averaged values are Recommended. At 298K the values cluster around two values: 0.019 (ref 1, 2, 6) and 0.016 g(1)/100g sln (ref 6, 7, 9, 11). Although the values of Bohon and Claussen (ref 2) in well characterized systems are often high this is not sufficient justification for favouring the lower values (ref 7, 9, 11) at this stage. At other temperatures,



COMPONENTS :	EVALUATOR:
<pre>(1) p-Xylene; C₈H₁₀; [106-42-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

agreement is equally poor and at higher temperatures (323-363K) only the values of Pryor and Jentoft (ref 3) are available. Clearly this system warrants further investigation. Selected data have been plotted in Figure 1 which emphasizes the differences among the available data.

Thermodynamic functions derived from various data sets by application of the van't Hoff equation are summarized in Table 3.

TABLE 3: Thermodynamic Functions for the Dissolution ofp-Xylene in Water Derived from Solubility Data

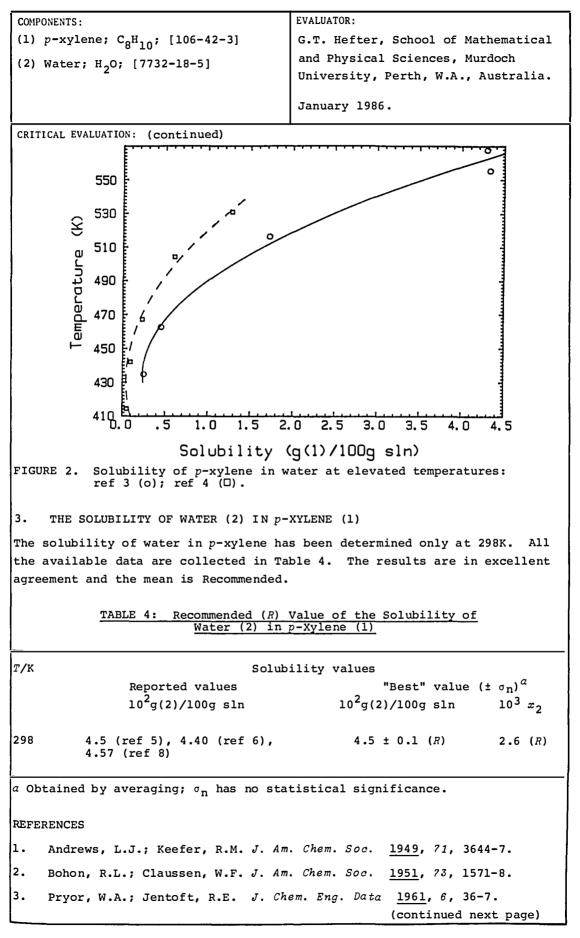
Reference	^{AH} sln kJ mol ⁻¹	^{AC} p,sln J K-1 mol-1
Bohon and Claussen (ref 2)	3.9	-211
Pryor and Jentoft (ref 3)	7.8^{a}_{b} 30.4 ^b	122 ^a 81 ^b
Guseva and Parnov (ref 4)	16.0	210
Sanemasa <i>et al</i> . (ref 11)	3.2	11
"Best" values (Table 2)	6.9	204

a 316 < T < 360 K b 434 < T < 568 L

Comparison of the thermodynamic data in Table 3 with similar but better characterized hydrocarbon systems (e.g. benzene in water) suggests that none of the solubility data for p-xylene in water are very reliable (including the "Best" values).

2. SOLUBILITY OF p-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for p-xylene in water at elevated temperatures (*ca.* 400-570K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of confirmatory data it is not possible to know which set is more reasonable. Thermodynamic functions derived from both data sets (Table 3) are in poor agreement and differ markedly from low T values. The interested user is referred to the relevant Data Sheets for the experimental values.



EVALUATOR: COMPONENTS: G.T. Hefter, School of Mathematical (1) p-Xylene; C₈H₁₀; [106-42-3] and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. January 1986 CRITICAL EVALUATION: (continued) REFERENCES (continued) 1963, 18, 76-9. 4. Guseva, A.N.: Parnov, E.I. Vestn. Mosk. Univ. Khim. Hoegfeldt, E.; Bolander, B. Ark. Kemi 1964, 21, 161-86. 5. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23. 6. 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. 8. Kirchnerova, J.; Cave, G.C.B. Can. J. Chem. 1976, 54, 3909-16. 9. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also Ph.D. Dissertation 1974, University of California, Riverside, CA, 1973, quoted in ref 22. U.S.A., Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7. 10. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62. 11.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3] (2) Water; H ₂ O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
(2) water; n_20 ; [7732-16-5]	9. An. Chem. 500. <u>1949</u> , 71, 5044-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of p-Xylene in water a	t 25°C was reported to be
0.0200 g(1)/100 g sln.	
The corresponding mole fraction, x_1 , calculated by the compilers is 3.39 x 10^{-5} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
A mixture of (1) and (2) was rotated	(1) Eastman Kodak Co. best grade;
for twenty hours in a constant tem- perature bath at 25 C. A sample	fractionally distilled; b.p. 138.5 C.
(5-20 mL) of the aqueous phase was	-
withdrawn and extracted with a measured volume of hexane (10-50 mL)	(2) Not specified.
by shaking in a glass stoppered Erlenmeyer flask. Next, the absorb-	
ance of the hexane phase was measured against a hexane blank on the	
Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Deben D.L. Cleveren M.D.
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Bohon, R.L.; Claussen, W.F.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem . Soc. <u>1951</u> , 73, 1571-8.
VARIABLES:	PREPARED BY:
Temperature: 0.4-42.8°C	G.T. Hefter
EXPERIMENTAL VALUES:	
	-xylene in water D0g sln ^a 10 ⁵ x1
	00g sln ^a 10 ⁵ x ₁ piler) (compiler)
	0156 ^b , 2.64 ^b
	0188 ^b 3.19 ^b
	0197 3.34 0195 3.31
	3.34
25.0 0.0	3.36 ^c
	3.37
	0201 3.41 0204 3.46
	0207 3.51
	3.51
42.8 0.0	3.76
^b Data refer to solubility solid (1) in ^c Given in the original paper as 0.1989	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A round-bottomed flask containing. about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of	refractometry (no details given). (2) Air-free conductivity water, no other details given.
the samples were inserted into a	ESTIMATED ERROR:
quartz cuvette and measured in a	Temp. ± 0.02°C
Beckman DU spectrophotometer. Absorbances were corrected for	Soly. ± 0.5% relative
adsorption of (1) onto the walls	
of the cuvette.	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Pryor, W.A.; Jentoft, R.E.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1961</u> , 6, 36-7.
VARIABLES:	PREPARED BY:
Temperature: 43.0-294.5°	A. Maczynski and Z. Maczynska

Solubility of p-xylene in water

	t/°C		3	
Cloud point appears	Cloud point disappears	Midpoint	10 ³ x1	g(l)/l00 g sln (compiler)
42.8	43.3	43.0	0.0434	0.0256
54.4	58.3	56.4	0.0510	0.0301
61.7	68.3	65.0	0.0576	0.0340
73.9	76.7	75.3	0.0656	0.0387
85.0	89.4	87.2	0.0779	0.0459
161.7	163.3	162.5	0.4264	0.2508
186.7	189.5	188.1	0.7686	0.4514
241.6	244.9	243.2	2.9555	1.7174
280.5	284.4	282.5	7.6238	4.3326
291.6	298.3	294.5	7.5407	4.2871

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dis- solved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud dis- appeared. The cycle was repeated three to four times until reliable appearance and disappearance temper- atures for the cloud were recorded.	<pre>(1) source not specified; 99.1% by freezing point; main impurities are isomeric xylenes; used as received. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES: </pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.
VARIABLES:	PREPARED BY:
Temperature: 141 - 258°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of p-	xylene in water
t/°C g(1)/100 g s	$\frac{10^4 x_1 \text{ (compiler)}}{10^4 x_1 \text{ (compiler)}}$
141 0.049	0.83
169 0.096 194 0.231	1.63 3.93
231 0.607 258 1.283	10.34
	22.00
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n _D ²⁰ 1.4958.
	(2) doubly distilled.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Hoegfeldt, E.; Bolander, B.
(2) Water; $H_{2}O;$ [7732-18-5]	Ark. Kemi, <u>1964</u> , 21, 161-86.
	<u> </u>
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of water in p-Xylene wa	as reported to 0.022 mol(2) L^{-1} sln.
The corresponding mass percent and mo	l fraction, x_2 , calculated by the
compilers are 0.045 g(2)/100 g sln and	1 0.0027.
The assumption that 1.00 L sln = 857 g	sln was used in the Calculation
	sin was used in the calculation.
AUXILIARY	INFORMATION
	SOURCE AND PURITY OF MATERIALS:
The water determination was carried out according to Johansson's modifi-	 Fluka; 0.04% of ethylbenzene; purity 99.8%; used as received.
cation of the Karl Fischer titration	
described in ref 1, 2.	(2) Not specified.
	ESTIMATED ERROR: Temp. ±0.3°C
	Soly. ±0.002 mol(2) L ⁻¹ sln (type of error not specified)
	REFERENCES:
	 Hardy, C.J.; Greenfield, B.F.; Scargill, D.
	J. Chem. Soc. <u>1961</u> , 90. 2. Johansson, A.
	Sv. Papperstidn. <u>1947</u> , 11B, 124.

(1) p-Xylene; $C_{gH_{10}}$; $[105-42-3]$ Polak, J.; Lu, B.CY. Can. J. Chem. <u>1973</u> , 51, 4018-23.(2) Water; H ₂ O; $[7732-18-5]$ Can. J. Chem. <u>1973</u> , 51, 4018-23.VARIABLES: Temperature: $0-25^{\circ}$ CA. Maczynski and Z. MaczynskaSolubility of p-xylene in water $t^{/^{\circ}}$ C of(a) $g(1)/kg(2)$ $g(1)/kg(2)$ $g(1)/l00$ g sln (compiler) c^{-1} (compiler) $(compiler)$ $o^{\dagger}(a)$ $164(c)$ 0.0164 2.78 25 (b) $185(c)$ 0.0185 3.14 The solubility of water in p-xylene at 25° C was reported to be 440 $mg(1)/kg(2)$.The corresponding mass percent and mole fraction, x_2 , calculated by the compilers are 0.0440 $g(2)/100$ g sln and 2.59×10^{-3} .AUXILARY INFORMATIONMURINARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILLARY INFORMATIONENTROMAPPARATUS/PROCEDURE:AUXILARY INFORMATIONENTROMAPPARATUS/PR	COMPONENTS:	ORIGINAL MEASUREMENTS:		
VARIABLES: Temperature: $0-25^{\circ}$ CPREFARED BY: A. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:EXPERIMENTAL VALUES: 2^{\prime}° Cmg(1)/kg(2)o†(a)164(c)0.01642.7825 (b)185(c)0.01653.14The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2).Automatic colspan="2">Automatic colspan="2">Colspan="2"Colspan="2"Colspan="2"Colspan="2"Author MaterialsColspan="2"Colspan="2"Colspan="2"Colspan="2"Colspan="2"Colspan="2"Colspan="2"Colspan="2"<	(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Polak, J.; Lu, B.CY.		
Temperature: 0-25°CA. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Solubility of p-xylene in water $t/°C mg(1)/kg(2) g(1)/l00 g sln lo5zi (compiler)(compiler) (compiler)$	(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1973</u> , 51, 4018-23.		
Temperature: 0-25°CA. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Solubility of p-xylene in water $t/°C mg(1)/kg(2) g(1)/100 g sln 10^5 x_1(compiler)$				
Temperature: $0-25^{\circ}C$ A. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Solubility of p-xylene in water $t'^{\circ}C$ $g(1)/kg(2)$ $g(1)/kg(2)$ $g(1)/kg(2)$ $(compiler)$ $($	VARIABLES:	DEFDADED BV.		
EXPERIMENTAL VALUES: Solubility of p-xylene in water $t/^{\circ}C$ mg(l)/kg(2) g(l)/l00 g sln 10 ⁵ x1 (compiler) (compiler) 0†(a) 164(c) 0.0164 2.78 25 (b) 185(c) 0.0185 3.14 The solubility of water in p-xylene at 25°C was reported to be 440 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_2 , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . a^{-C} See "Estimated Error" †p-xylene was at supercooled liquid state. AUXILIARY INFORMATION NETROD/APPARATUS/PROCEDURE: Approvimately 50 mL of (1) together with (2) were placed in a 125 mL Ethop coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 2 dh rad left in the bath for 3 days or was kept in the control the ba				
Solubility of p-xylene in water $t/^{\circ}C$ mg(1)/kg(2)g(1)/100 g sln $10^{5}x_{1}$ (compiler)0†(a)164(c)0.01642.7825 (b)185(c)0.01853.14The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2).The corresponding mass percent and mole fraction, x_{2} , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10^{-3} .AUXILIARY INFORMATIONMETHOD/AFPARATUS/PROCEDURE:AUXILIARY INFORMATIONMETHOD/AFPARATUS/PROCEDURE:ADDOT (1) together with (2) were placed in a 25° mL placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath for 3 days or three water layer was determined by Karl Fischer titration and the solubi	Temperature: 0-25 C	A. Maczynski and Z. Maczynska		
t/°C mg(1)/kg(2) g(1)/100 g sln 10 ⁵ x1 0†(a) 164(c) 0.0164 2.78 25 (b) 185(c) 0.0185 3.14 The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2). The corresponding mass percent and mole fraction, x2, calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . AUXILIARY INFORMATION See "Estimated Error" †p-xylene was at supercooled liquid state. SOURCE AND PURITY OF MATERIALS: AUXILIARY INFORMATION Source AND PURITY OF MATERIALS: Aution organics, pure grade with distilled water. (2) distilled.	EXPERIMENTAL VALUES:			
a-c See "Estimated Error" tp-xylene was at supercooled liquid state. a-c See "Estimated Error" tp-xylene was at supercooled liquid state. AUXILIARY INFORMATION METROD/APPARATUS/FROCEDURE: Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a taflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by gas bitter first first in and the water layer was determined by gas	Solubility of p-	xylene in water		
25 (b) 185(c) 0.0185 3.14 The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_2 , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Auxiliant in the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . Summeter are 0.0410 to g sln and 2.59 x 10 ⁻³ .	t/°C mg(1)/kg(2) g(1)	$1)/100 \text{ g sln}$ $10^5 x_1$ (compiler) (compiler)		
The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2). The corresponding mass percent and mole fraction, x ₂ , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . a ^{-C} See "Estimated Error" †p-xylene was at supercooled liquid state. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the water layer was determined by gas	0†(a) 164(c)	0.0164 2.78		
440 mg(1)/kg(2). The corresponding mass percent and mole fraction, x ₂ , calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59 x 10 ⁻³ . a-c See "Estimated Error" †p-xylene was at supercooled liquid state. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Pischer titration and the solubility of hydrocarbon in the water layer was determined by gas Auxiliant of the system was determined by gas	25 (b) 185(c)	0.0185 3.14		
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.(1) Eastman Organics, pure grade reagent; shaken three times with distilled water.(2) distilled.(2) distilled.ESTIMATED ERROR: temp. (a) ± 0.02°C, (b) ± 0.01°C soly. (c) ± 1.7% (from two or three determinations)	^{a-c} See "Estimated Error"			
 Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas abromatography. (1) Eastman Organics, pure grade reagent; shaken three times with distilled water. (2) distilled. (2) distilled. (2) distilled. (3) ESTIMATED ERROR: (4) ± 0.02°C, (b) ± 0.01°C soly. (c) ± 1.7% (from two or three determinations) 	AUXILIARY	INFORMATION		
<pre>with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas abromategraphy</pre>	METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:			
	with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas	 (1) Eastman Organics, pure grade reagent; shaken three times with distilled water. (2) distilled. ESTIMATED ERROR: temp. (a) ± 0.02°C, (b) ± 0.01°C soly. (c) ± 1.7% (from two or three determinations) 		

00_00	
COMPONENTS: (1) p-Xylene; C ₈ H ₁₀ ; [106-42-3] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Kirchnerova, J.; Cave, G.C.B. Can. J. Chem. <u>1974</u> , 54, 3909-16.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
The solubility of water in p-xylene 0.0217 mol(2)/L and $x_2 = 0.00269$. T calculated by the compilers is 0.045	he corresponding mass percent

AUXILIARY	INFORMATION
UDVIDIUUI	THEOREMITON

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was emersed up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days. The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Fisher 277; purified by double crystallization.
- (2) not specified.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.0002 mol(2) dm⁻³ sln
(standard deviation from 5
determinations).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of p-xylene in water	at 25°C was reported to be
156.0 mg(1)/kg(2). The correspondin	g mass percent and mole fraction,
x_1 , calculated by the compilers are	0.01560 g(l)/100 g sln and
2.65×10^{-5} .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2)	(1) Aldrich Chemical Co. or
was determined by gas chroma- tography.	Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	<pre>temp. ± 0.1°C soly. 1.6 mg(1)/kg(2) (the standard deviation of the rear for give prolimeters)</pre>
	mean for six replicates) REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C and at system pressure was reported to be 157.0 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0157 g(l)/ 100 g sln and 2.66 x 10⁻⁵.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

 Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR: temp. ± 1°C

soly. ± 1.0 mg(1)/kg(2)

COMPONENTS:

(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413 - 7.
L	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
-	
EXPERIMENTAL VALUES:	
The solubility of p-xylene in water a	at 25°C was reported
to be 157.0 mg(1)/kg(2).	-
The corresponding mass percent and mo	ble fraction, $x_{1,j}$ calculated
by compiler are 0.0157 g(1)/100 g slr	- <u>-</u>
2] COMPTEE and COULDY 3(1),100 9 21	
Editor's Note: Based on the results	for this and other hydrocarbon-water
systems, uncertainity exists about wh	_
independent of that of Price for the	same system (see previous page).
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in	(1) not specified.
(2) were prepared in two ways. First, 200 近 of (1) was injected	(2) not specified.
into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	
and (2) as above was thermostatted at 70°C and then cooled to 25°C. The	
time required to obtain equilibrium was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
ograph equipped with a $100-150-mesh$ Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat- urated solutions of heptane in (2)	soly. 3.9 mg(l)/kg(2) (standard
were used as standard solutions.	deviation from 7-9 determinations).
	REFERENCES:

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

50_42	51	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) p-Xylene; C ₈ H ₁₀ ; [106-42-3] (2) Water; H ₂ O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.	
VARIABLES:	PREPARED BY:	
Temperature: 15-45°C	G.T. Hefter	
EXPERIMENTAL VALUES:		
The solubility of	p-xylene in water	
t/°C 10 ³ mol(1)/dm ³ sln	g(l)/l00 g sln $10^5 x_1$ (compiler) ^a (compiler) ^a	
15 1.48 ^b	0.0157 2.67	
25 1.53 ± 0.07	0.0163 2.76	
35 1.61 ± 0.08	0.0172 2.92	
45 1.66 ± 0.05	0.0178 3.02	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory		
funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.	soly. see table, type of error not	

1. Kell, G.S.
 J. Chem. Eng. Data <u>1975</u>, 20, 97.

 Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. <u>1981</u>, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(l) p-Xylene; C ₈ H ₁₀ ; [106-42-3]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref l)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of p-xylene in artifi	
110.9 mg(1)/kg sln. The correspondi	
_	01109 g(1)/100 g sln and 1.93 x 10^{-5}
assuming the artificial seawater com	position of ref 1.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.
chromatography.	
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.9 (std. dev.)
	REFERENCES: 1. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.
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COMPONENTS:	EVALUATOR:
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of theEthylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Fühner (ref 1)	288	(l) in (2)	titration
Andrews and Keefer (ref 2)	298	(l) in (2)	spectrophotometric
Klevens (ref 3)	298	(l) in (2)	spectrophotometric
Bohon and Claussen (ref 4)	273-316	(l) in (2)	spectrophotometric
Filippov and Furman (ref 5)	291-323	(2) in (l)	synthetic
Morrison and Billett (ref 6)	298	(l) in (2)	analytical
Jones and Monk (ref 7)	298-308	(2) in (1)	radiotracer
McAuliffe (ref 8)	298	(l) in (2)	GLC
Guseva and Parnov (ref 9)	338-507 ^a	(l) in (2)	unspecified
Englin <i>et al</i> . (ref 10)	283-303	(2) in (1)	analytical
McAuliffe (ref ll)	298	(l) in (2)	GLC
Polak and Lu (ref 14)	273,298	mutual	GLC, Karl Fischer
Brown and Wasik (ref 15)	278-293	(l) in (2)	chromatographic
Sutton and Calder (ref 16)	298	(l) in (2)	GLC
Price (ref 17)	298	(l) in (2)	GLC
Korenman and Aref'eva (ref 1	8) 293	(l) in (2)	titration
Korenman and Aref'eva (ref l	9) 298	(l) in (2)	titration
Krzyzanowska and Szeliga (ref 20)	298	(l) in (2)	GLC
Sanemasa <i>et al</i> . (ref 21,22)	288-318	(l) in (2)	spectrophotometric
Sanemasa <i>et al</i> . (ref 23)	298	(l) in (2)	spectrophotometric
Heidman <i>et al</i> . (ref 24)	311-568 ^a	mutual	GLC, Karl Fischer

a Pressure also varied, see Table 6.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Critical phenomena at high pressures have been reported by Alwani and Schneider (ref 12) and Roof (ref 13) and are discussed along with the high pressure solubility data (ref 9, 24) in Section 3 below. For convenience, further discussion of this system will be divided into three parts.

COMPONENTS:	EVALUATOR:
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

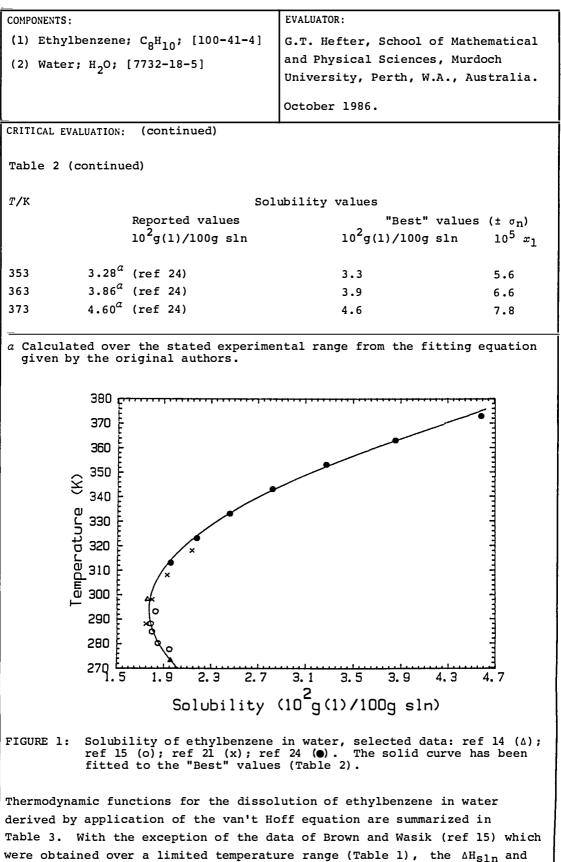
In the tables which follow values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original authors' experimental data. "Best" values have been obtained by averaging all non-rejected data. Standard deviations (σ_n) have been included as a convenient measure of the spread of experimental results: they do not have any statistical significance.

1. SOLUBILITY OF ETHYLBENZENE (1) IN WATER (2)

Of the data available on the solubility of ethylbenzene in water, values of Bohon and Claussen (ref 4) and Korenman and Aref'eva (ref 18) have been rejected because they are significantly higher (by about 10%) than all other studies. The value of Price (ref 17) at 298K is markedly lower than all other studies and is also rejected. The datum of Krzyzanowska and Szeliga (ref 20) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 17). The remaining data are summarized in Table 2 and are generally in excellent agreement even though few studies have covered the same temperature range (which has limited the number of Recommended values). Selected data are also plotted in Figure 1.

T/K	Solubilit	y values		
Reported values	Reported values	"Best" values (± σ_n)		
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	10 ⁵ <i>x</i> 1	
273	1.97 (ref 14)	2.0	3.4	
283	1.84* (ref 15)	1.8	3.1	
293	1.84* (ref 15), 1.77 (ref 21)	1.81 ± 0.04 (R)	3.07 (<i>R</i>)	
298	<pre>1.68 (ref 2), 1.75 (ref 3), 1.65 (ref 6), 1.59 (ref 8), 1.52 (ref 11), 1.77 (ref 14), 1.61 (ref 16), 1.8 (ref 19), 1.81 (ref 21), 1.69 (ref 22), 1.72 (ref 23)</pre>	1.69 ± 0.09 (R)	2.87 (<i>R</i>)	
303	1.86* (ref 21)	1.9	3.2	
313	2.03* (ref 21), 1.97 ^{<i>a</i>} (ref 24)	$2.00 \pm 0.03 (R)$	3.39 (R)	
323	2.19 ^{<i>a</i>} (ref 24)	2.2	3.7	
333	2.47 ^a (ref 24)	2.5	4.2	
343	2.83 ^{α} (ref 24)	2.8	4.8	

TABLE 2:	Recommended	(R) and	Tentative	Values	of	the	Solubility
	of Et	hylbenze	ne (1) in	Water ((2)		



 $\Delta C_{p,sln}$ derived from the various values are quite close to reliable calorimetric values reported for the dissolution of benzene in water. This gives added confidence to the solubility data in Table 2. (continued next page)

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COMPONENTS:

(1) Ethylbenzene; C<sub>8</sub>H<sub>10</sub>; [100-41-4]

(2) Water; H<sub>2</sub>O; [7732-18-5]

University, Perth, W.A., Australia.

October 1986.
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CRITICAL EVALUATION: (continued)

<u>TABLE 3: Thermodynamic Functions for the Dissolution of</u> <u>Ethylbenzene in Water Derived from Solubility Data</u>

Reference	^{∆H} sln kJ mol-1	^{AC} p,sln J K ⁻¹ mol ⁻¹
Brown and Wasik (ref 15)	11.9	1123
Sanemasa et al. (ref 21)	3.6	319
Sanemasa et al. (ref 22)	3.9	230
Heidman et al. (ref 24)	4.5	213
"Best" values (Table 2)	2.1	275

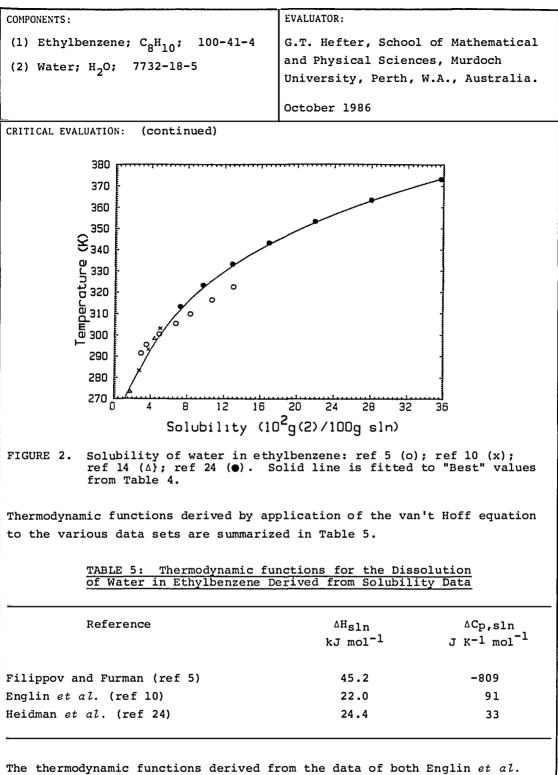
2. SOLUBILITY OF WATER (2) IN ETHYLBENZENE (1)

With the exception of the data of Jones and Monk (ref 7) which are reported in v/v fractions, all the available values for the solubility of water in ethylbenzene are summarized in Table 4 below. Unfortunately, few of the determinations cover the same temperature range. Where comparison is possible at lower temperatures ($T \le 298$ K) independent determinations are in reasonable agreement. At higher temperatures (T > 298K) the values of Filippov and Furman (ref 5) and Heidman *et al.* (ref 24) show an increasing divergence with increasing temperature (Figure 2).

TABLE 4: Recommended (R) and Tentative Values of the Solubilityof Water (2) in Ethylbenzene (1)

T/K	Solubilit	y values	
	Reported values	"Best" valu	
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	$10^{3} x_{2}$
273	1.78 (ref 14)	1.8	1.1
283	2.75 (ref 10)	2.8	1.7
293	3.3* (ref 5), 3.73 (ref 10)	3.5 ± 0.2	2.1
298	4.2* (ref 5), 4.4* (ref 10), 4.42 (ref 14)	4.3 ± 0.1 (R)	2.5 (R)
303	5.9* (ref 5), 5.02 (ref 10)	5.5 ± 0.5	3.2
313	9.6* (ref 5), 7.2 $^{\alpha}$ (ref 24)	8 ± 1	5
323	13.3* (ref 5), 9.68 ^{<i>a</i>} (ref 24)	11 ± 2	6
333	12.9 ^{<i>a</i>} (ref 24)	13	8
343	16.9 ^{<i>a</i>} (ref 24)	17	10
353	21.9 ^{<i>a</i>} (ref 24)	22	13
363	28.0 ^{<i>a</i>} (ref 24)	28	17
373	35.6 ^{<i>a</i>} (ref 24)	36	21

a Calculated over the stated experimental range by the fitting equation given by the original authors. (continued next page)



The thermodynamic functions derived from the data of both Englin *et al.* (ref 10) and Heidman *et al.* (ref 24) are comparable to those obtained for related, well characterized systems (*e.g.* water in benzene) whereas the values of Filippov and Furman (ref 5) are not. Further investigation of this system is clearly warranted.

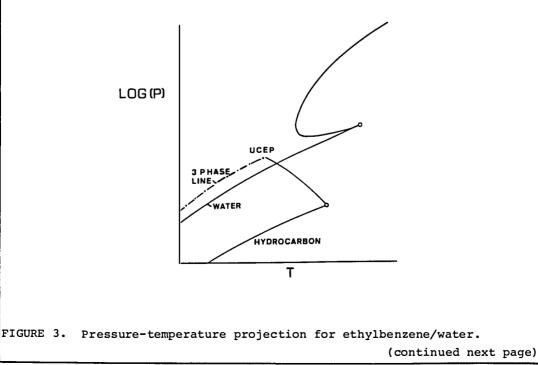
COMPONENTS:	EVALUATOR:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.
	October 1986.

CRITICAL EVALUATION: (continued)

3. MUTUAL SOLUBILITIES OF ETHYLBENZENE (1) AND WATER (2) AT ELEVATED TEMPERATURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram for this system. On such a diagram (Figure 3) phases with the same value of pressure and temperature but different composition will be located at the same point. The general typology of the phase diagram of this system is similar to that of benzene + water (except that the vapor pressure of ethylbenzene is considerably less than that of benzene). Ethylbenzene + water has type III phase behaviour (using Scott and von Konynenberg's classification (ref 25, 26). This type of phase behaviour is characterized by two critical loci, with one starting at the critical point of the pure component with the higher critical temperature (water in this case) and eventually approaching high pressures. The other critical locus starts at the critical point of the other pure component (ethylbenzene) and ends on a three phase (liquid-liquid-vapor) line at a critical end point.

The p-T projection of the p-T-x diagram for this system is shown schematically in Figure 3.



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COMPONENTS :	EVALUATOR:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

It is important to note that the three phase line on a p-T projection corresponds to three lines on the p-T-x diagram. In the region above the three phase line on the p-T projection, the pressure is greater than the vapor pressure and then a maximum of two liquid phases is possible. There may be one or two liquid phases depending on the overall composition. To the left of the critical line starting at the least volatile component it is possible to have one or two phases present depending on the overall composition.

Solubilities in the ethylbenzene + water system have been studied at elevated pressures in the publications listed in Table 6.

Reference	p/kPa	<i>т/</i> к	Solubility
Guseva and Parnov (ref 9)	_a	338-507	(1) in (2)
Alwani and Schneider (ref 12)	1.8-2.0	348-387	critical locus
Roof (ref 13)			- ^b
Heidman <i>et al</i> . (ref 24)	0.1-10.7 [°]	311-568	mutual

 TABLE 6:
 Solubility Studies of the Ethylbenzene (1) - Water (2)

 System at Elevated Pressures

a Unspecified but presumably at pressures on the three phase line.

b Critical point of unknown composition.

c Along three phase line.

The data of Guseva and Parnov (ref 9) are thought to be unreliable. The solubilities reported by these workers are considerably larger than values obtained by other workers for the systems water + benzene, + hexane, + ethylcyclohexane and + octane. The data of Heidman *et al.* (ref 24) are classified as Tentative for measurements along the three phase line. However, it should be pointed out that there is some discrepancy between the critical end point properties (574.3K, 11.2 MPa) reported by Roof (ref 13) and those reported by Heidman *et al.* (568.1K, 10.68 MPa). Nevertheless, the thermodynamic functions derived from the data of Heidman *et al.* (Table 3) and also with those of related hydrocarbons (*e.g.* benzene in water).

Alwani and Schneider (ref 12) have reported values of the critical properties along the critical curve starting at the critical point of ethylbenzene (cf. Figure 3).

(continued next page)

COMPONENTS: EVALUATOR: G.T. Hefter, School of Mathematical (1) Ethylbenzene; C₈H₁₀; [100-41-4] and Physical Sciences, Murdoch University, Perth, W.A., Australia. (2) Water; H₂O; [7732-18-5] October 1986 CRITICAL EVALUATION: (continued) REFERENCES 1. Fühner, H. Chem. Ber. 1924, 57, 510-5. 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, 72, 5034-7. Klevans, H.B. J. Phys. Chem. 1950, 54, 283-98. 3. 4. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8. 5. Filippov, T.S.; Furman, A.A. Zh. Prikl. Khim. 1952, 25, 895-7. 6. Morrison, T.J.; Billett, F. J. Chem. Soc. 1952, 3819-22. 7. Jones, J.R.; Monk, C.B. J. Chem. Soc. 1963, 2633-5. McAuliffe, C. Nature 1963, 200, 1092-3. 8. 9. Guseva, A.N.; Parnov, E.I. Zh. Fiz. Khim. 1964, 38, 805-6. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6. 10. 11. McAuliffe, C. J. Phys. Chem. 1966, 70, 1267-75. 12. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. 1969, 70, 294-301. 13. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23. 14. Brown, R.L.; Wasik, S.P. J. Res. Natl. Bur. Stds. A. 1974, 78, 453-60. 15. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. 16. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also 17. Ph.D. Dissertation, Univ. California, Riverside, CA, U.S.A., 1973, quoted in ref 22. 18. Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977,04.05. Korenman, I.M.; Aref'eva, R.P. 2h. Prikl. Khim. 1978, 51, 957-8. 19. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7. 20. 21. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Chem. Lett. 1981, 225-8. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 22. <u>1982</u>, 55, 1054-62. Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc. 23. Jpn. 1984, 57, 1539-44. 24. Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. A.I.Ch.E.J. <u>1985</u>, *31*, 376-84. Scott, R.L.; van Konynenburg, P.H. Phil. Trans. Roy. Soc., London 25. 1980, A298, 495. 26. Hicks, C.P.; Young, C.L. Chem. Rev. 1975, 75, 119.

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38_45	67
Components:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Fuhner, H.
(2) Water; H ₂ O; [7732-18-5]	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
VARIABLES:	PREPARED BY:
One temperature: 15°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat 0.014 g(1)/100 g sln.	er at 15°C was reported to be
The corresponding mole fraction, x_1 , c_2 .4 x 10^{-5} .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts	 Source not specified; commer- cial grade; used as received.
of (1) were added with shaking to 50, 100, or 1000 cm ³ (2) until a completely clear solution was no longer obtained at the experimental temperature.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
	<u> </u>
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wate	er at 25°C was reported to be
0.0168 g(1)/100 g sln.	
The corresponding mole fraction, x_1 , (2.85×10^{-5}) .	calculated by the compilers is
2.85 x 10 ⁻ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated	(1) Eastman Kodak Co. white label;
for twenty hours in a constant tem- perature bath at 25°C. A sample	fractionally distilled; b.p. 136.0°C.
(5-20 mL) of the aqueous phase was	-
withdrawn and extracted with a measured volume of hexane (10-50 mL)	(2) Not specified,
by shaking in a glass stoppered Erlenmeyer flask. Next, the absorb-	
ance of the hexane phase was mea-	
sured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS :	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat 0.175 g(1) L^{-1} sln and 0.00164 mol(1	er at 25°C was reported to be) L ⁻¹ sln.
The corresponding mass percent and mo compiler are 0.0175 g(1)/100 g sln an	
1	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.
of (1) in 1 liter of (2) for as long	(2) not specified.
as three months. Aliquots were removed and concentrations deter-	
mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

7	1	٦
1	٠	J

70	38_48
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Bohon, R.L.; Claussen, W.F.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8.
-	
VARIABLES:	PREPARED BY:
Temperature: 0.4-42.8°C	G.T. Hefter
EXPERIMENTAL VALUES:	
	ylbenzene in water
	$\begin{array}{ccc} 00 \text{g sln}^{a} & 10^{5} x_{1} \\ \text{npiler}) & (\text{compiler}) \end{array}$
	0219 3.71
5.2 0.	0213 3.61
	0207 3.51 0207 3.51
	0208 ^b 3.53
	0209 3.54 0211 3.58
	0211 3.58 0221 3.75
	0231 3.92 orted as "optical density" (absorbance)
Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(l)/l00g sln by assumi ^b Given in the original paper as 0.208	rities) and corrected optical of g(l)/L sln which was then ng a solution density of 1.00 kg/L.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.	

38_470		71
COMPONENTS:		ORIGINAL MEASUREMENTS:
<pre>(1) Ethylbenzene; C (2) Water; H₂O; [77</pre>		Filippov, T.S.; Furman, A.A. <i>Zh. Prikl. Khim.</i> <u>1952</u> , 25, 895-7.
VARIABLES:		PREPARED BY:
Temperature: 18.2-	49.5°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:		
s	olubility of water	n ethylbenzene
t/°C	g(2)/100 g slm	$\frac{10^3 x_2}{2}$ (compiler)
18.2	0.0296	1.74
18.3	0.0308	1.81
19.7 22.3	0.0327 0.0352	1.92 2.07
23.4	0.0360	2.12
24.2	0.0388	2.28
27.2	0.0494	2.91
29.8	0.0595	3.50
31.6 32.1	0.0648 0.0679	3.81 4.05
34.2	0.0745	4.38
35.1	0.0777	4.56
36.6	0.0835	4.90
38.8	0.0917	5.38
41.5 43.1	0.1005 0.1070	5.90 6.27
47.2	0.1225	7.18
49.5	0.1300	7.62

AUXILIARY INFORMATION

İ	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	Weighed amounts of both components were placed in glass tubes, 40 mm across and 65 mm long, and shaken. Clear and cloud points were ob- served 5-6 times to within 0.2- 0.3°C.	 (1) source unspecified; distilled; no turbidity if cooled to -10 or -20°C. (2) twice distilled.
		ESTIMATED ERROR:
		temp: ± 0.3°C soly: not specified
		REFERENCES:

72	38_49
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Morrison, T.J.; Billett, F.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1952</u> , 3819-22.
VARIABLES :	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in war 0.00155 mol(1)/1000 g(2). The corresponding mass percent and mo by compilers are 0.0165 g(1)/100 g si	ole fraction, x_1 , calculated
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
After an excess of (1) had been shaken with about 1 dm^3 of (2) for about a week, a known volume of saturated solution was made slightly	(1) source not specified; purest obtainable material; distilled; purity not specified.
alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in	(2) not specified.
soda-asbestos. The precautions usual in organic combustions were taken.	ESTIMATED ERROR: temp. ± 0.1°C soly. ± 1% (mean of large numbers of determinations)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Jones, J.R.; Monk, C.B.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1963</u> , 2633-5.
2	
VARIABLES:	PREPARED BY:
Temperature: 25-35°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
Solubility of Wa	ter in Ethylbenzene
t/°C	10^4 mL (2)/mL (1)
25	3.7
30 35	4.3 5.3
33	2.2
AUXILIAR	Y INFORMATION
AUXILIAR METHOD/APPARATUS/PROCEDURE :	Y INFORMATION SOURCE AND PURITY OF MATERIALS;
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a	SOURCE AND PURITY OF MATERIALS; (1) Laboratory grade; dried over CaCl ₂ and fractionally distille
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali-	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distille
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter-	 SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distille (2) Not specified.
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	 SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distille (2) Not specified.
	 SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl₂ and fractionally distille (2) Not specified.
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND FURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distille (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1%
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distiller (2) Not specified. ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1%
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND PURITY OF MATERIALS; (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1% (average deviation)
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND PURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distilled (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1% (average deviation)
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL ali- quot was reshaken for 4 hrs. with 5 mL H ₂ O in a 10 mL flask, sampled and assayed with a Nuclear Enter- prises type 8301 liquid scintillation counter. The two-stage process eli- minates quencing effects (due to	SOURCE AND FURITY OF MATERIALS: (1) Laboratory grade; dried over CaCl ₂ and fractionally distille (2) Not specified. ESTIMATED ERROR: Soly. ±5% to ±1% (average deviation)

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) 1963, 200, 1092-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat 0.0159 g(l)/100 g sln.	
The corresponding mole fraction, x_1 , 2.70 x 10 ⁻⁵ .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon- saturated water was injected directly into a gas liquid chromatograph.	ESTIMATED ERROR:
	Temp. ±1.5°C Soly. 0.0008 (std. dev. of mean) REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. 1964, 38, 805-6.
2	
VARIABLES:	PREPARED BY:
Temperature: 115.0 - 233.5°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of ethylbe	nzene in water
	2.04
t/°C g(1)/100 g sln	$10^4 x_1$ (compiler)
115.0 0.0513	0.871
140.5 0.119	2.02
170.5 0.355 210.0 0.661	6.04 11.27
233.5 1.129	19.33
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in	(1) not specified.
sealed glass tubes. No details	
were reported in the paper.	(2) not specified.
	ESTIMATED ERROR:
	not specified.
	not specificu.
	REFERENCES:
1	

ORIGINAL MEASUREMENTS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , <i>10</i> , 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wate	er in Ethylbenzene
<u>t/°C</u> g(2)/100 g sli	$\frac{10^3 x_2 (compiler)}{10^3 x_2 (compiler)}$
100.0275200.0373300.0502	1.62 2.19 2.95
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.
	ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wat to be 152 g(1)/10 ⁶ g(2). The corresponding mass percent and mo by the compilers are 0.0152 g(1)/100	ble fraction, x_1 , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<pre>(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 8 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:</pre>

77

COMPONENTS:			ORIGINAL MEASUREME	NTC .
(1) Ethylbe	enzene; C ₈ H ₁₀ ; [100-	•41-4]	Polak, J.; Lu,	B.CY.
(2) Water;	H ₂ O; [7732-18-5]		Can. J. Chem.	<u>1973</u> , <i>51</i> , 4018-23.
VARIABLES:			PREPARED BY:	
Temperature: 0-25°C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL V	ALUES:			
	Solubility	of eth	ylbenzene in wa	ter [.]
t/°C	mg(1)/kg(2))/100 g sln compiler)	$10^4 x_1$ (compiler)
0(a)	197(c)		0.0197	3.34
25 (b)	177(c)		0.0177	3.00
	Solubility	y of wat	er in ethylbenz	ene
<i>t/</i> °C	mg(2)/kg(1))/100 g sln compiler)	$10^{3}x_{2}$ (compiler)
0(a)	178(d)		0.0178	1.05
25 (b)	442(e)		0.0442	2.60

Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR: temp. (a) \pm 0.02°C, (b) \pm 0.01°C soly. (c) \pm 1.7%, (d) \pm 4.7%, (e) \pm 3.1% (from two or three determinations)

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) F thylbonzono, C H , [100-41-4]	Brown, R.L.; Wasik, S.P.
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	
(2) Water; H ₂ O; [7732-18-5]	J. Res. Natl. Bur. Stds. A. <u>1974</u> , 78, 453-60.
VARIABLES :	PREPARED BY:
Temperature: 4.5-20.1°C	G.T. Hefter
EXPERIMENTAL VALUES:	
Solubility of Eth	ylbenzene in Water
	-
<u>t/°C g(l)/100 g sl</u>	n^{a} $10^{5} x_{1}$ (compiler)
4.5 0.0196 ± 0.00 6.3 0.0192 ± 0.00	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2.16
	05 5.07
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	05. 3.12 04 ^b 3.1
20.1 0.018 ± 0.00	04 J.L
<i>a</i>	
^a Errors given as standard deviations	
^b Typographical error in original pub decimal place.	fication, digit missing in fourth
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were calculated from	(1) 99.99 mole per cent purity;
Partition coefficient measurements for the hydrocarbon between an	source and methods of purifi- cation not specified.
aqueous solution and its vapor using headspace chromatography. The appa-	(2) Distilled.
ratus and the method of obtaining the	
partition coefficients are described in detail in the paper. Basically,	
the hydrocarbon was introduced as a vapor (to avoid emulsification) into	
a glass equilibration cell containing	
about 45 cm of water. The vapor was subsequently analysed by gas chroma-	ESTIMATED ERROR:
tography using He as the carrier. Possible sources of error are dis-	Temperature: ±0.01°C
cussed in detail although the source of vapor pressure data used to calcu-	Solubility: See Table above.
late solubilities are not given.	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Eng. Data 1975, 20,
	320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 161.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01612 g(1)/100 g sln and 2.734 x 10⁻⁵.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	<pre>temp. ± 0.1°C soly. 0.9 mg(1)/kg(2) (the standard deviation of the</pre>
	mean for six replicates) REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C and at system pressure was reported to be 131.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0131 g(1)/ 100 g sln and 2.22 x 10⁻⁵.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de-	 SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
tails are given in the paper.	ESTIMATED ERROR: temp. ± 1°C soly. ± 1.4 mg(1)/kg(2) REFERENCES:

81

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Korenman, I.M.; Aref'eva, R.P.
(2) Water; H ₂ O; [7732-18-5]	Patent USSR, 553 524, 1977.04.05 C.A. <i>87</i> :87654.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski
EXPERIMENTAL VALUES:	

The solubility of ethylbenzene in water at 20°C was reported to be 0.21 g(1) L^{-1} (2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.021 g(1)/100 g sln and 3.6 x 10⁻⁵. The assumption that 1 dm³ sln = 1 kg sln was used in the calculation.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

38_60	83
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Korenman, I.M.; Aref'eva, R.P.
(2) Water; H ₂ O; [7732-18-5]	Zh. Prikl. Khim. 1978, 51, 957-8.
2	
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in wate 0.18 g(l) L ⁻¹ sln.	er at 25°C was reported to be
The corresponding mass percent and moto compilers are 0.018 g(1)/100 g sln and 1.00 $L^{-1} = 1.00$ kg sln was used in the	$1 3.1 \times 10^{-5}$. The assumption that
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 200-500 mL (2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).	(1) Not specified.(2) Not specified.

ESTIMATED ERROR:

Soly. 0.01 g(1) L⁻¹ sln (std. dev. from 6 deter-minations).

84	38_63
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	•
The solubility of ethylbenzene in water at 25°C was reported to be 131.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 0.0131 g(1)/100 g sln and 2.22 x 10 ⁻⁵ .	
Editor's Note: Based on the results systems, uncertainity exists about w	for this and other hydrocarbon-water hether the datum compiled here is
independent of that of Price for the	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

The saturated solutions of (1) in (2) were prepared in two ways. (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-ll gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat-urated solutions of heptane in (2) were used as standard solutions.

- (1) not specified.
- (2) not specified.

ESTIMATED ERROR:

soly. 3.4 mg(1)/kg(2) (standard deviation from 7-9 determinations).

COMPONENTS:	· · · · · · · · · · · · · · · · · · ·	ORIGINAL MEASUREMENTS:	
(l) Ethylbenzene	; C ₈ H ₁₀ ; [100-41-4]	Sanemasa, I.; Arak Nagai, H.	i, M.; Deguchi, T.;
(2) Water; H ₂ O;	[7732-18-5]	Chem. Lett. <u>1981</u> ,	225-8.
VARIABLES:		PREPARED BY:	
Temperature: 15-	45°C	M.C. Haulait-Pirso	n
EXPERIMENTAL VALUES:			
	Solubility of eth	ylbenzene in water	
t/°C	g(1)/L	g(l)/100 g sln ^a	$10^{4}x_{1}^{a}$
15	0.176 ± 0.009	0.0176	2.99
25			3.09
35	0.194 ± 0.006	0.0195	3.31
45	0.215 ± 0.004	0.0217	3.69
the sam			
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PRO		INFORMATION SOURCE AND PURITY OF M	IATERIALS :
METHOD/APPARATUS/PRO The apparatus us	CEDURE: ed for attaining	SOURCE AND PURITY OF M (1) analytical rea	WATERIALS: Igent grade used as
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the	CEDURE: ed for attaining ibrium is described paper. Liquid (1)	SOURCE AND PURITY OF M (1) analytical rea purchased.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added.	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	igent grade used as
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled.	igent grade used as
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro spectrophotometr chloroform extra	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in ic measuring the cts were not reported	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR: soly. : given abov	igent grade used as
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro spectrophotometra The solubility r	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in ic measuring the	SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled. ESTIMATED ERROR: soly. : given abov REFERENCES: 1. CRC Handbook of	re Chemistry and
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro spectrophotometr chloroform extra The solubility r that the tempera voir was made to	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in ic measuring the cts were not reported uns were made such ture of solute reser- vary while that of	<pre>SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled. (2) redistilled. ESTIMATED ERROR: soly. : given abov REFERENCES: 1. CRC Handbook of Physics, R.C. W CRC Press, Flor</pre>	re Chemistry and east, Editor,
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro spectrophotometr chloroform extra The solubility r that the tempera voir was made to soluvent phase wa solubility obeys	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in ic measuring the cts were not reported uns were made such ture of solute reser- vary while that of s held constant. The Henry's law at con-	<pre>SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled. (2) redistilled. ESTIMATED ERROR: soly. : given abov REFERENCES: 1. CRC Handbook of Physics, R.C. W CRC Press. Flor</pre>	re Chemistry and east, Editor,
METHOD/APPARATUS/PRO The apparatus us solubility equil in detail in the and redistilled vessel and a the respectively. T erated by bubbli liquid solute wa funnel and circu pump. The circu min. Solubility attained within of 10 mL of the transferred into mL of chloroform Experimental pro spectrophotometr chloroform extra The solubility r that the tempera voir was made to solvent phase wa	CEDURE: ed for attaining ibrium is described paper. Liquid (1) (2) were placed in a rmostatted funnel he solute vapor, gen- ng air through the s introduced into the lated by means of a lation rate was 2 L/ equilibria were 5 min. Then portions aqueous sln were funnels to which 10 had been added. cedures involved in ic measuring the cts were not reported uns were made such ture of solute reser- vary while that of s held constant. The Henry's law at con- mperature. Solubil-	<pre>SOURCE AND PURITY OF M (1) analytical rea purchased. (2) redistilled. (2) redistilled. ESTIMATED ERROR: soly. : given abov REFERENCES: 1. CRC Handbook of Physics, R.C. W CRC Press, Flor</pre>	re Chemistry and east, Editor,

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Sanemasa, I.; Araki, M.;
0 10	
(2) Water; H ₂ O; [7732-18-5]	Deguchi, T.; Nagai, H.
	Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.
VARIABLES:	PREPARED BY:
	G.T. Hefter
Temperature: 15-45°C	G.I. HEILEI
EXPERIMENTAL VALUES:	
The solubility of et	hylbenzene in water .
$t/^{\circ}$ C 10 ³ mol(1)/dm ³ sln	$g(1)/100 g sln = 10^5 x_1$
	(compiler) ^a (compiler) ^a

2.72 15 1.51 ± 0.08 0.0160 25 2.87 1.59 ± 0.05 0.0169 35 1.54 ± 0.05 0.0176 2.99 0.0196 3.33 45 1.83 ± 0.05

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.	 Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification. Redistilled; no further details given.
	ESTIMATED ERROR:
	<pre>soly. see table, type of error not specified. temp. ± 0.01°C.</pre>
weight fiom pure fiquid soluces.	REFERENCES:
	 Kell, G.S. <i>J. Chem. Eng. Data</i> <u>1975</u>, 20, 97. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. <i>Chem. Lett.</i> <u>1981</u>, 225-8.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5]</pre>	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. <i>Bull. Chem. Soc. Jpn.</i> <u>1984</u> , <i>57</i> , 1539-44.
VARIABLES:	PREPARED BY:
One Temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be $1.62 \times 10^{-3} \mod(1)/\text{dm}^3 \text{ sln.}$ Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 0.0172 g(1)/100 g sln, $x_1 = 2.92 \times 10^{-5}$, calculated by the compiler.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculat- ing pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed	 Analytical reagent grade source and purity not stated, used without further purification. Deionized and redistilled; no further details given. 	
by solvent extraction - UV spectro- photometry.		
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES :	
	 Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62. 	

COMPONENTS:

<pre>(1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water, H₂O; [7732-18-5]</pre>	Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. <i>A. I. Ch. E. J.</i> <u>1985</u> , <i>31</i> , 376-84.
VARIABLES: Temperature: 311-568 K Pressure: 0.01-10.7 MPa	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

р /МРа	$10^4 x_1$	g(l)/100 g sln (compiler)
_ a	0.32	0.019
0.111	0.86	0.051
0.627	2.19	0.129
2.32	6.0	0.35
6.50	32.5	1.88
8.59	37.5	2.17
	_ a 0.111 0.627 2.32 6.50	$ \begin{array}{c} -a & 0.32 \\ 0.111 & 0.86 \\ 0.627 & 2.19 \\ 2.32 & 6.0 \\ 6.50 & 32.5 \end{array} $

a Not specified.

(continued)

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.	purity ≥99.9 mol %, checked
	<pre>ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. REFERENCES: 1. Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. <u>1983</u>, 29, 990-9.</pre>

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(1) Ethylbenzene; C<sub>8</sub>H<sub>10</sub>; [100-41-4]
(2) Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

Solubility of water in ethylbenzene

<i>т </i> к	р /МРа	10 ² x ₂	g(2)/100 g sln (compiler)
310.9	0.0091 ^{<i>a</i>}	0.43	0.073
367.6	0.111	1.86	0.320
423.4	0.627	5.96	1.06
479.5	2.32	16.3	3.20
536.1	6.50	40.8	10.5
550.4	8.27	47.2	13.2
568.1 ^b	10.68 ^b	69.1 ^b	27.5

a Estimated by the authors from pure component data.

b Three phase critical point.

The three phase critical point was reported to be 568.1 \pm 0.6 K, 10.68 \pm 0.04 MPa and $x_1 = 5.83 \times 10^{-3}$ (3.34 g(1)/100 g sln, compiler).

The authors also report an equation providing a fit of their own and literature data over the range 273-568 K, viz.

 $\ln x_1 = -185.1695 + 7348.55/T + 26.34525 \ln T$ $\ln x_2 = -0.37215 - 4.4626 (T_p^{-1} - 1) - 0.38596 (1 - T_p)^{1/3}$ $- 2.59850 (1 - T_p)$

where $T_r = T/568.1$

COMPONENTS:		ORIGINAL	MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ;	[100-41-4]	Brown	, R.L.; Wasik, S.P.
(2) Artificial seawater			s. Natl. Bur. Stds. A. <u>1974</u> , 53-60.
VARIABLES:		PREPARED) BY:
Temperature: 0-20°C		G.T.	Hefter and D.G. Shaw
Salinity: 34.42 g salts/k	g sln		
EXPERIMENTAL VALUES:			
Solubility of	ethylbenzen	e in ar	tificial seawater
<u>t/°C</u>	g(l)/100 g	sln ^a	$10^{5}x_1$ (compiler)
0.19	0.0140 (0.0	002)	2.44
5.32	0.0133 (0.0	0031	2.31
10.05	0.0129 (0.0	003)	2.25
	0.0125 (0.0		2.18
20.04	0.0122 (0.0	003)	2.12
	AUXILIARY	INFORMAT	TION
METHOD/APPARATUS/PROCEDURE:		SOURCE	AND PURITY OF MATERIALS:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of ob- taining the partition coefficients	(2)	99.99 mole per cent purity; source and methods of purifi- cation not specified. Prepared according to ref 1. Purity not specified.	
are described in detail in The hydrocarbon was introd vapor (to avoid emulsifica a glass equilibration cell	the paper. luced as a tion) into containing		
about 45 L of water. The subsequently analysed by g	-		ED ERROR:
graphy using He as the car Possible sources of error	rier.	Tempe	rature: ±0.01 K ility: see Table above
cussed in detail although	the source	Solub	
	the source d to cal-	REFEREN 1. Sv Fl Pr	

COMPONENTS:

(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of ethylbenzene in ar lll.0 mg (1)/kg sln. The correspond x_1 calculated by the compiler are 0. assuming the artificial seawater comp	ing mass percent and mole fraction, 01110 g(1)/100 g sln and 1.9 x 10^{-5}
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.	 SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure.
	ESTIMATED ERROR: temp. ± 0.1°C soly. 1.3 (std. dev.) REFERENCES: 1. Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u> , 3, 135.
1WW 2-H	

ORIGINAL MEASUREMENTS:

(1) Ethylbenzene; C₈H₁₀; [100-41-4] Sutton, C.; Calder, J.A.

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<pre>S2 COMPONENTS: (1) 4-Vinyl-1-cyclohexene; C₈H₁₂; [100-40-3] (2) Water; H₂O; [7732-18-5] VARIABLES: One temperature: 25°C EXPERIMENTAL VALUES: The solubility of 4-vinyl-1-cyclohexe to be 50 g(1)/10⁶ g(2). The corresponding mass percent and mc by the compilers are 0.005 g(1)/100 g </pre>	ORIGINAL MEASUREMENTS: McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75. PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski ene in water at 25°C was reported ple fraction, x ₁ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1)	(1) Phillips Petroleum or

ESTIMATED ERROR:

temp.	± 1.5°C _
soly.	$\frac{1}{5} g(1) / 10^{6} g(2)$
	(standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Propenylcyclopentane; C ₈ H ₁₄ ; [5623-78-9]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
One temperature: 30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of water in 1-propenyl reported to be 0.0383 g(2)/100 g sln. mole fraction, x_2 , calculated by the	The corresponding value
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Octyne; C ₈ H ₁₄ ; [629-05-0]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 1-octyne in water a to be 24 g(1)/10 ⁶ g(2). The corresponding mass percent and mo by the compilers are 0.0024 g(1)/100	ble fraction, x_1 , calculated
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton	 (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
syringe and gas liquid chromato- graphed in conjunction with a flame-	ESTIMATED ERROR:
ionization detector.	<pre>temp. ± 1.5°C soly. 0.8 g(1)/10⁶ g(2)</pre>
	REFERENCES :

COMPONENTS: (1) 1,1,3-Trimethylcyclopentane; C ₈ H ₁₆ ; [4516-69-2] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.	
VARIABLES: PREPARED BY: One temperature: 25°C M.C. Haulait-Pirson		
EXPERIMENTAL VALUES: The solubility of 1,1,3-trimethylcyclopentane in water at 25°C and at system pressure was reported to be 3.73 mg(1)/kg(2).		

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 3.73 x 10⁻⁴ g(1)/100 g sln and 5.99 x 10⁻⁷.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were car- ried out by GLC using a Hewlett- Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+8. (2) Distilled.</pre>	
	ESTIMATED ERROR: Temp. ±1°C Soly. ±0.17 mg(l)/kg(2)	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,1,3-Trimethylcyclopentane;</pre>	Krzyzanowska, T.; Szeliga, J.
C ₈ H ₁₆ ; [4516-69-2] (2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclopentane in water at 25°C was reported to be 2.04 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 2.04 x 10^{-4} g(1)/100 g sln and 3.27 x 10^{-7} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	ESTIMATED ERROR: soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Isopropylcyclopentane; C₈H₁₆; [3875-51-2]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

Solubility of water in	isopropylcyclopentane
------------------------	-----------------------

<i>t</i> /°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.0059	3.68
20	0.0102	6.35
30	0.0159	9.90

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) not specified.(2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES :

98	38_74
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Propylcyclopentane; C₈H₁₆; [2040-96-2] Water; H₂O; [7732-18-5] 	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of propylcyclopentane system pressure was reported to be 2. corresponding mass percent and mole of by the compiler are 2.04 x 10 ⁻⁴ g(1),	.04 mg(l)/kg(2). The fraction, x ₁ , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	 (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR:
	<pre>temp. ± 1°C soly. ± 0.10 mg(1)/kg(2)</pre>
	REFERENCES:

38_75

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylcyclopentane; C ₈ H ₁₆ ;	Krzyzanowska, T.; Szeliga, J.
[2040-96-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

The solubility of propylcyclopentane in water at 25°C was reported to be 1.77 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 1.77 x 10^{-4} g(1)/100 g sln and 2.84 x 10^{-7} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.

100	38_76	
COMPONENTS: (1) cis-1,2-Dimethylcyclohexane; C ₈ H ₁₆ ; [2207-01-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.	
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski	
EXPERIMENTAL VALUES: The solubility of cis-1,2-dimethylcyclohexane in water at 25°C was reported to be 6.0 g(1)/10 ⁶ g(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00060 g(1)/100 g sln and 9.6 x 10 ⁻⁷ .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.8 g(1)/10⁶ g(2) (standard deviation of mean)</pre>	

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 1,4-Dimethylcyclohexane; C₈H₁₆; [589-90-2]</pre>	Guseva, A.N.; Parnov, E.I.	
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>196</u> 19, 77 - 8.	<u>.4</u> ,
VARIABLES:	PREPARED BY:	į
Temperature: 57-240°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of 1,4-dimeth	ylcyclohexane in water	
t/°C g(l)/100 g(2)	g(1)/100 g sln 10 ⁴ a (compiler) (compil	21 .er)
57 0.0017	0.0017 0.02	.7
105 0.0056	0.0056 0.09	0
165 0.0263	0.0263 0.42	
240 0.257	0.257 4.12	0
<u> </u>		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Presumably the measurements were made in sealed glass tubes, as	(1) not specified.	
reported in ref 1. No more details were reported in the paper.	(2) not specified.	
	ESTIMATED ERROR:	
	ESTIMATED ERROR: not specified.	
	not specified.	<u>1963</u> ,
	<pre>not specified. REFERENCES: 1. Guseva, A.N.; Parnov, E.I Vestn. Mosk. Univ. Khim.</pre>	<u>1963</u> ,

COMPONENTS :	ORIGINAL MEASUREMENTS:	
 1,4-trans-Dimethylcyclohexane; C₈H₁₆; [2207-04-7] Water; H₂O; [7732-18-5] 	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 1,4-trans-dimethylcyclohexane in water at 25°C and at system pressure was reported to be 3.84 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 3.84 x 10^{-4} g(l)/100 g sln and 6.16 x 10^{-7} .		

AUXILIARY	AUXILIARY INFORMATION		
AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 0.17 mg(l)/kg(2) REFERENCES:		

COMPONENTS :	ORIGINAL MEASUREMENTS:
 1,4-Dimethylcyclohexane; C₈H₁₆; 	Krzyzanowska, T.; Szeliga, J.
[589-90-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,4-dimethylcyclohexane in water at 25°C was reported to be 3.84 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 3.84 x 10^{-4} g(1)/100 g sln and 6.16 x 10^{-7} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	(1) not specified.(2) not specified.
ograph equipped with a 100-150 mesh	ESTIMATED ERROR:
Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<pre>soly. 0.12 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>
	REFERENCES:

CRITICAL EVALUATION:

104

Quantitative solubility data for the ethylcyclohexane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies.of theEthylcyclohexane (1) - Water (2) System

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	352-486	(l) in (2)	unspecified ^a
Heidman <i>et al</i> . (ref 2)	311-561	mutual	GLC, Karl Fischer

a Probably using the synthetic method.

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system is in two parts.

1. SOLUBILITY OF ETHYLCYCLOHEXANE (1) IN WATER (2)

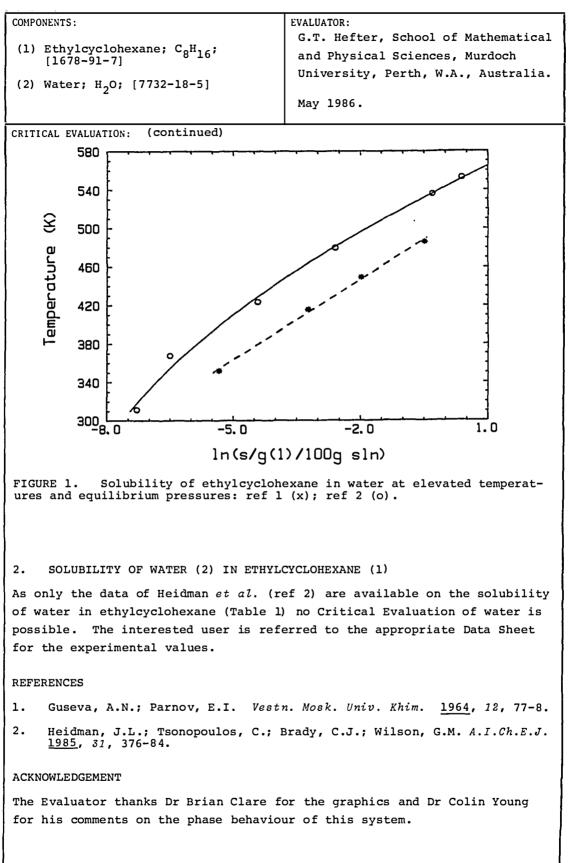
This system almost certainly exhibits type III phase behaviour (see introductory material at the beginning of this volume). The phase diagram is similar to that of ethylbenzene and water.

The solubility of ethylcyclohexane in water at elevated temperatures and system pressures along the three phase equilibrium line have been investigated by Guseva and Parnov (ref 1) and Heidman *et al.* (ref 2). Their results are summarized in Table 2 and plotted in Figure 1. The agreement is very poor. However, it may be noted (ref 1) that the values reported by Guseva and Parnov at higher temperatures approach those of cyclohexane which is unreasonable. It may also be noted that the data of Guseva and Parnov often differ markedly from Recommended values in other systems. The data of Heidman *et al.* are thus considered Tentative.

Heidman *et al*. report a three phase critical end point at 561.4 \pm 0.6 K, 9.93 \pm 0.04 MPa and x_1 = 3.35 x 10⁻³ (2.05 g(1)/100g sln, Evaluator).

COMPONEN	TS:	EVALUATOR:	
[10	hylcyclohexane; C ₈ H ₁₆ ; 578-91-7] ter; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mat and Physical Sciences, Mun University, Perth, W.A., A May 1986.	doch
CRITICAL	EVALUATION: (continued)		
TABLE 2: Tentative Solubility Values for Ethylcyclohexane (1) in Water (2) at the Three-Phase Equilibrium Pressure			
<i>т/</i> к		ubility values	Ъ
	Reported values ^a	"Best" value	
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	10 ⁴ x1
313	0.066 (ref 2)	0.07	0.01
323	0.074 (ref 2)	0.07	0.011
333	0.086 (ref 2)	0.07	0.014
343	0.10 (ref 2)	0.10	0.016
353	0.5 (ref 1), 0.13 (ref 2)	0.13	0.020
363	0.8 (ref 1), 0.16 (ref 2)	0.16	0.026
373	1.3 (ref 1), 0.21 (ref 2)	0.21	0.034
393	2.2 (ref 1), 0.55 (ref 2)	0.55	0.088
413	3.7 (ref 1), 0.95 (ref 2)	0.95	0.15
433	6.5 (ref 1), 1.6 (ref 2)	1.6	0.26
453	16.0 (ref 1), 2.8 (ref 2)	2.8	0.45
473	27.0 (ref 1), 5.5 (ref 2)	5.5	0.9
493	16 (ref 2)	16	2.2
513	34 (ref 2)	34	5.2
533	65 (ref 2)	65	10.4
	150 (ref 2)	150	24.0

a All data obtained by graphical or algebraic interpolation by the Evaluator of the authors' original data.
b Rounded values from ref 2; data from ref 1 not included in "Best" values, see text.



COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Ethylcyclohexane; C ₈ H ₁₆ ;	Guseva, A.N.; Parnov, E.I.	
	Vestn. Mosk. Univ. Ki 19, 77-8.	nim. <u>1964</u> ,
(2) Water; H ₂ O; [7732-18-5]	19, 77-8.	
VARIABLES:	PREPARED BY: M.C. Haulait-Pirson	
Temperature: 79-213°C	M.C. haulait-filson	
EXPERIMENTAL VALUES:	······································	
Solubility of ethylcy	clohexane in water	
t/°C g(1)/100 g(2)	g(l)/100 g sln (compiler)	$10^4 x_1$ (compiler)
79 0.0048	0.0048	0.077
142.5 0.0398	0.0398	0.639
176 0.138 213 0.66	0.138 0.62	2.22 9.96
213 0.66	0.02	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATER	RIALS:
Presumably the measurements were made in sealed glass tubes, as	(1) not specified.	
reported in ref 1. No more details were reported in the paper.	(2) not anonified	
	(2) not specified.	
were reported in the paper.	(2) not specified.	
were reported in the paper.	(2) not specified.	
were reported in the paper.	(2) not specified.	
were reported in the paper.		
were reported in the paper.	ESTIMATED ERROR:	
were reported in the paper.		
were reported in the paper.	ESTIMATED ERROR: not specified.	
were reported in the paper.	ESTIMATED ERROR:	
were reported in the paper.	ESTIMATED ERROR: not specified. REFERENCES: 1. Guseva, A.N.; Par Vestn. Mosk. Unit	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylcyclohexane; C ₈ H ₁₆ ;	Heidman, J.L.; Tsonopoulos, C.;
[1678-91-7]	Brady, C.J.; Wilson, G.M.
(2) Water, H ₂ O; [7732-18-5]	A. I. Ch. E. J. <u>1985</u> , 31, 376-84.
VARIABLES: Temperature: 311-561 K Pressure: 0.01-9.9 MPa	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

	Solubility of	ethylcyclohexane i	n water
<i>т </i> к	p /MPa	10 ⁴ x ₁	10 ² g(l)/100 g sln (compiler)
311.5	a	0.011	0.068
367.6	0.117	0.024	0.15
423.4	0.647	0.20	1.2
479.5	2.36	1.21	7.5
536.1	6.69	11.8	73
552.8	8.83	23.7	146

a Not specified.

(continued)

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observ- ation. This aspect of the procedure is discussed in detail in the paper.	 SOURCE AND PURITY OF MATERIALS: (1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography. (2) Distilled; no details given.
	ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. REFERENCES: 1. Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. <u>1983</u> , 29, 990-9.

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(1) Ethylcyclohexane, C<sub>8</sub>H<sub>16</sub>; [1678-91-7]
(2) Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

Solubility of water in ethylcyclohexane

<i>Т </i> К	р /МРа	10 ² x ₂	g(2)/100 g sln (compiler)
310.9	0.0099 ^a	0.081	0.0130
367.6	0.117	0.65	0.104
423.4	0.647	3.0	0.48
479.5	2.36	10.7	1.89
536.1	6.69	29.0	6.15
552.8	8.83	41.4	10.2
561.4 ^b	9.93 ^b	60.3 ^b	19.6

a Estimated by the authors from pure component data.

b Three phase critical point.

The three phase critical point was reported to be 561.4 \pm 0.6 K, 9.93 \pm 0.04 MPa and $x_1 = 3.35 \times 10^{-3}$ (1.05 g(1)/100 g sln, compiler).

The authors also report an equation which fits their own and related literature data over the range 273-561 K, viz.

 $\ln x_1 = -334.2468 + 14105.21/T + 47.93102 \ln T$ $\ln x_2 = -0.50980 - 7.4603 (T_p^{-1} - 1) - 0.67885 (1 - T_p)^{1/3}$ $+ 0.44796 (1 - T_p)$

where $T_{p} = T/561.4$

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclooctane; C ₈ H ₁₆ ; [292-64-8]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. 1966, 70, 1267-75.
(2) water, n_20 , $[7752 \pm 0.5]$	<u> </u>
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
one temperature: 25 C	M.C. Hadiait Filson
EXPERIMENTAL VALUES:	
The solubility of cyclooctane in wate	r at 25°C was reported to
be 7.9 mg (1)/kg sln.	

The corresponding mole fraction, x_1 , calculated by the compiler, is 1.27 x 10^{-6} . The same value is also reported in ref 1.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
In a 250 mL glass bottle, $10-20$ mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	<pre>(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 1.8 mg (1)/kg sln (standard deviation from mean)</pre>	
	REFERENCES: 1. McAuliffe, C. Am. Chem. Soc. Div. Petrol. Chem. <u>1964</u> , 9, 275.	

38_84

ORIGINAL MEASUREMENTS: McAuliffe, C.
McAuliffe, C.
J. Phys. Chem. <u>1966</u> , 70, 1267-75.
PREPARED BY:
A. Maczynski, Z. Maczynska, and A. Szafranski
at 25°C was reported ole fraction, x_1 , calculated 0 g sln and 4 x 10^{-7} .
INFORMATION
SOURCE AND PURITY OF MATERIALS:
 (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.2 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:

112	38_85
COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Octene; C₈H₁₆; [111-66-0] (2) Water; H₂0 [7732-18-5]</pre>	Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data <u>1972</u> , 17, 328-9
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson, G.T. Hefter
EXPERIMENTAL VALUES:	
by the compilers are respectively, 0	
^a It should be noted that although t	be authors state that the solubility

It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol L^{-1} HNO₃ solution.

AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted	<pre>(1) Matheson, Coleman and Bell; 99%</pre>
glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard	(2) Not specified
procedures.	
	ESTIMATED ERROR:
	Temp. ± 0.05K Soly. not specified.
	REFERENCES :

Components :	ORIGINAL MEASUREMENTS:
(1) 2-Octene; C ₈ H ₁₆ ; [111-67-1] (2) Water; H ₂ O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data <u>1972</u> , 17, 328-9.
VARIABLES:	PREPARED BY:
Temperature: 15-25°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 2-octene in 0.001 mol/L $\rm HNO_3$ solution.

t/°C	10 ⁴ mol/L sln ^a	10 ³ g(l)/100 g sln ^b (compiler)	10 ⁶ ¤ ₁ (compiler)
15	2.92 ± 0.14	3.3	5.3
20	2.51 ± 0.16	2.8	4.5
25	2.16 ± 0.15	2.4	3.9

a Uncertainties stated to be "standard deviations from means".

b Assuming a solution density of 1.00 g mL⁻¹ at all temperatures.

<u>Compiler's note</u>: Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause olefin Solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol L^{-1} HCl.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After Settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard Procedures.	 Prepared by dehydration of 2-octanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. Not specified.
	ESTIMATED ERROR:
	Temp. ± 0.05 K Soly. see table above.
	REFERENCES :

COMPONENTS :	EVALUATOR:
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

			<u> </u>
Reference	T/K	Solubility	Method
Berkengeim (ref l)	273-313	(2) in (1)	Karl Fischer
Baker (ref 2)	unspecified	(l) in (2)	radiotracer
Englin <i>et al</i> . (ref 3)	273-323	(2) in (1)	analytical
McAuliffe (ref 4)	298	(l) in (2)	GLC
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Budantseva <i>et al</i> . (ref 6)	293	mutual	unspecified
Price (ref 7)	298	(l) in (2)	GLC
Krzyzanowska and Szeliga (ref 8)	298	(l) in (2)	GLC

TABLE 1: Quantitative Solubility Studies of the 2,2,4-Trimethylpentane (1) - Water (2) System

The original data in all of these publications are compiled in the Data Sheets immediatley following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,2,4-TRIMETHYLPENTANE (1) IN WATER (2)

Very few data are available for the solubility of 2,2,4-trimethylpentane in water making critical evaluation difficult. The datum of Baker (ref 2) is rejected as the temperature was not specified. All other reported values are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 8) which does not appear to be independent of that of Price (ref 7) and has therefore been excluded from consideration.

At 298K where comparisons are possible, the values of McAuliffe (ref 4) and Polak and Lu (ref 5) are in reasonable agreement. The value reported by Price (ref 7) is much lower. Although Price's data for many hydrocarbons in water are normally reliable, many of his values for the higher hydrocarbons are lower than other studies. However, in the absence of confirmatory studies it is not reasonable to reject Price's value at this stage. However, it has not been included in the calculation of the "Best" values at 298K.

At other temperatures the "Best" values should be regarded with caution in the absence of confirmatory studies. (continued next page)

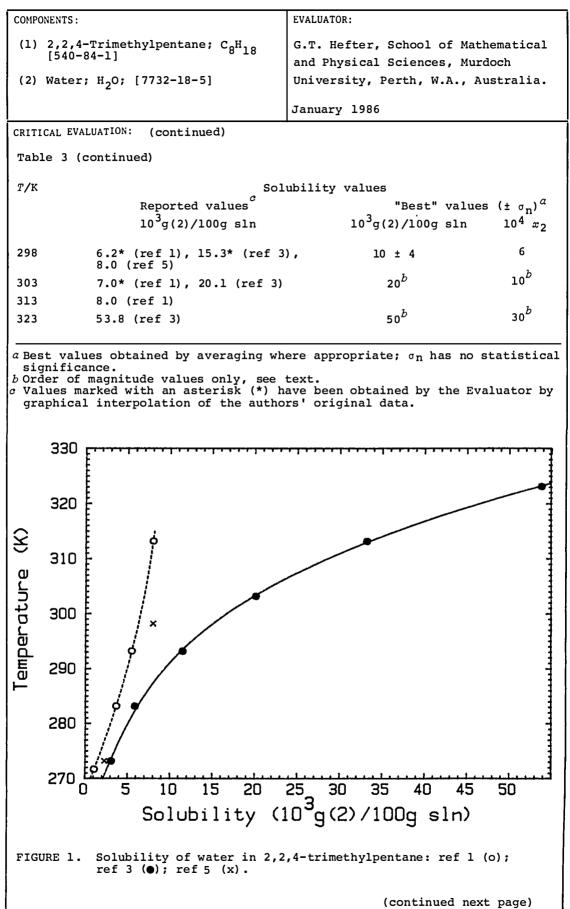
			11
COMPONENTS :		EVALUATOR:	
(1) 2,2,4-Tr [540-84-	rimethylpentane; C ₈ H ₁₈ ;	G.T. Hefter, School of Math	nematical
	-	and Physical Sciences, Murc	loch
(2) water; i	H ₂ O; [7732-18-5]	University, Perth, W.A., Au	stralia.
		January 1986.	
CRITICAL EVALU	ATION: (continued)		
	TABLE 2: Tentative Value 2,2,4-Trimethylpenta	es of the Solubility of ane (1) in Water (2)	
T/K	Solu	bility values	
1	Reported values	"Best" values	
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x ₁
273 2	2.46 (ref 5)	2.5	3.9
293 2	2 (ref 6)	2	3
	2.44 (ref 4), 2.05 (ref 5) 1.14 (ref 7)	2.2 ± 0.2^{b}	3.5 ^b
cance.	data from ref 4 and 5 onl	ate; σ _n has no statistical s .y, see text.	igniii-
		-	
2. SOLUBII	ITY OF WATER (2) IN 2,2,4-	TRIMETHYLPENTANE (1)	
	reported values of the sol collected in Table 3 and p	ubility of water in 2,2,4-tr blotted in Figure 1.	imethyl-
The data are	e generally in poor agreeme	ent and the averaged "Best" v	values
		further studies. Generally,	
other system	other systems investigated by these authors, the data of Englin <i>et al</i> .		
(ref 3) are reliable at T < 300K but are too high at higher temperatures.			
Application of the van't Hoff equation to the data of Englin $et \ al$. and			
Bergengeim (ref 1) gives values of $\Delta H_{sln} = 41.9$ and 20.1 kJ mol ⁻¹ and $\Delta C_{p,sln} = -100$ and -1950 J K ⁻¹ mol ⁻¹ respectively. Comparison of these			
L			
	data with other systems suggests that the values of Englin <i>et al</i> . are more realistic (although probably high at $T > 300$ K). This system clearly		
	ther investigation.		-1
TABLE 3: Tentative Values of the Solubility of			
Water (2) in 2,2,4-Trimethylpentane (1)			
<i>Т/</i> К	Solu	bility values	
	Reported values	"Best" values	
	10 ³ g(2)/100g sln	10 ³ g(2)/100g sln	104 ^x 2
	.7* (ref 1), 3.1 (ref 3), .3 (ref 5)	2.4 ± 0.6	1.5
283 3	.7 (ref 1), 5.9 (ref 3), .5* (ref 5)	4.7 ± 0.9	2.9

5.5 (ref 1), 11.5 (ref 3), 6.5* (ref 5), 7.9 (ref 6)

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(Table 3 continued next page)

8 ± 2



COMPONENTS :	EVALUATOR:	
<pre>(1) 2,2,4-Trimethylpentane; C_gH₁₈;</pre>	G.T. Hefter, School of Mathematical	
[540-84-1]	and Physical Sciences, Murdoch	
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.	
	January 1986.	
CRITICAL EVALUATION: (continued)		
REFERENCES		
1. Berkengeim, T.I. Zavod. Lab. 19	<u>941</u> , <i>10</i> , 592-4.	
2. Baker, E.G. Geochim. Cosmochim.	Acta <u>1960</u> , <i>19</i> , 309-17.	
 Englin, B.A.; Plate, A.F.; Tugolu Khim. Tekhnol. Topl. Masel <u>1965</u> 	nkov, V.M.; Pyranishnikova, M.A. , 10, 42-6.	
4. McAuliffe, C. J. Phys. Chem. 19	<u>966</u> , 70, 1267-75.	
5. Polak, J.; Lu, B.CY. Can. J. (Chem. <u>1973</u> , 51, 4018-23.	
 Budantseva, L.A.; Lesteva, T.M.; 50, 1344, Deposited doc. 1976, Vi 	Nemtsov, M.S. Zh. Fiz. Khim. <u>1976</u> , INITI 437-76.	
7. Price, L.C. Am. Assoc. Petrol.	Geol. Bull. <u>1976</u> , 60, 213-44.	
8. Krzyzanowska, T.; Szeliga, J. N	afta (Katowice) <u>1978</u> , 34, 413-7.	
ACKNOWLEDGEMENT		
The Evaluator thanks Dr Marie-Claire H	Haulait-Pirson for comments and	
Dr Brian Clare for the graphics and re	egression analyses.	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	; Berkengeim, T.I.
(2) Water; H ₂ O; [7732-18-5]	Zavod. Lab. <u>1941</u> , 10, 592-4.
VARIABLES:	PREPARED BY:
Temperature: (-1.5) - 40°C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubilitv of water i	in 2,2,4-trimethylpentane
t/°C g(2)/100	g sln $10^4 x_2$ (compiler)
$ \begin{array}{cccc} -1.5 & 0.00 \\ 10 & 0.00 \\ 20 & 0.00 \\ 40 & 0.00 \\ \end{array} $	037 2.35 055 3.49
	LARY INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; d²⁰_D0.6947; used as received. (2) not specified.</pre>
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

38_471	119	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]</pre>	Baker, E.G.	
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.	
VARIABLES:	PREPARED BY:	
One temperature: not specified	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 2,2,4-trimethylpent to be 0.0009 mL(1) L^{-1} (2).	tane in water was reported	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The procedure is described in ref 1.	not specified.	
	ECTIMATED EDDOD	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

1.	Baker	r, E.G.	Am.	Che	em.	Soc	ر ۱
	Div.	Petrol.	Cher	m.,	Pre	epri	nts
		, 3, N°4				-	

120	38_89		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.		
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
VARIABLES:	PREPARED BY:		
Temperature: 0-50°C	A. Maczynski and M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
Solubility of water in 2,	,2,4-trimethylpentane		
<u>t/°C</u> <u>g(2)/10</u>	$\frac{10^4 x_2}{(\text{compiler})}$		
0 0.0	1.97		
10 0.0	3.74		
20 0.0	0115 7.29		
30 0.0	12.74		
40 0.0	21.02		
50 0.0	34.03		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.		

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ; [540-84-1] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.	
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson	
EXPERIMENTAL VALUES: The solubility of 2,2,4-trimethylpentane in water at 25°C was reported to be 2.44 mg (1)/kg sln. The corresponding mole fraction, x_1 , calculated by the compiler, is 3.85 x 10 ⁻⁷ .		

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	 (1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.12 mg (1)/kg sln (standard deviation from mean) 	
	 REFERENCES: 1. McAuliffe, C. Nature (London) 1963, 200, 1092. 2. McAuliffe, C. Am. Chem. Soc., Div. Petrol. Chem. <u>1964</u>, 9, 275. 	

COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1] (2) Water; H₂O; [7732-18-5]</pre>	Polak, J.; Lu, B.C-Y. <i>Can. J. Chem.</i> <u>1973</u> , <i>51</i> , 4018-23.		
VARIABLES:	PREPARED BY:		
Temperature: 0-25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES: Mいいしょ	ت راه در ا		
Solubility of 2,2,4-trin	nethylpentane in water		
t/°C mg(l)/kg	sln <u>x₁ (compiler)</u>		
0 ^a 2.46 ^c 25 ^b 2.05 ^c	_		
Solubility of water in 2,2,4-trimethylpentane			
t/°C mg(2)/kg	sln x ₂ (compiler)		
0 ^a 23 ^d 25 ^b 80 ^e	1.46×10^{-4} 5.07 x 10^{-4}		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titra- tion. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetical- ly for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.	 (1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled. 		
	ESTIMATED ERROR: temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean) REFERENCES:		

COMPONENTS: ORIGINAL MEASUREMENTS:		
 (1) 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1] (2) Water; H₂O; [7732-18-5] Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. <i>Zh. Fiz. Khim.</i> <u>1976</u>, 50, 1344. Deposited doc. <u>1976</u>, VINITI 437-76. 		
VARIABLES: PREPARED BY:		
One temperature: 20°C A. Maczynski		
EXPERIMENTAL VALUES:		
The solubility of 2,2,4-trimethylpentane in water at 20°C was reported to be $x_1 = 3 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is about 2 x $10^{-4}g(1)/100$ g sln. The solubility of water in 2,2,4-trimethylpentane at 20°C was reported to be $x_2 = 4.4 \times 10^{-4}$. The corresponding mass percent value calculated by the compiler is 7.9 x 10^{-3} (2)/100 g sln.		
AUXILIARY INFORMATION		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing specified in the paper.	(1) not specified.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

38_93
ORIGINAL MEASUREMENTS:
Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
PREPARED BY:
M.C. Haulait-Pirson
cane in water at 25° C to be 1.14 mg(1)/kg(2). The fraction, x_1 , calculated /100 g sln and 1.80 x 10^{-7} .
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 0.02 mg(1)/kg(2) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C ₈ H ₁₈ ;	Krzyzanowska, T.; Szeliga, J.
[540-84-1]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,2,4-trimethylpen	tane in water at 25°C was reported
to be 1.14 mg(1)/kg(2).	
The corresponding mass percent and m	ole fraction, x_1 , calculated
by compiler are $1.14 \times 10^{-4} g(1)/100$	g sln and 1.80×10^{-7} .
-	_
Editor's Note: Based on the results	for this and other hydrocarbon-water
systems, uncertainity exists about w	-
independent of that of Price for the	same system (see previous page).
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in	(1) not specified.
(2) were prepared in two ways. First, 200 µL of (1) was injected	(2) not specified.
into 20 mL of (2) and thermostatted	_
at 25°C. Second, the mixture of (1) and (2) as above was thermostatted	
at 70°C and then cooled to 25°C. The time required to obtain equilibrium	
was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
ograph equipped with a 100-150 mesh	ESTIMATED ERROR:
Porasil column (70°C) and a flame ionization detector was used. Sat-	
urated solutions of heptane in (2) were used as standard solutions.	<pre>soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations).</pre>
	REFERENCES:

COMPONENTS:		EVALUATOR:
	<pre>(1) 2,3,4-Trimethylpentane; C₈H₁₈; [565-75-3] (2) Water; H₂0; [7732-18-5]</pre>	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
		February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,3,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1:	Quantitative	Solubility	Studie	s of the
2,3,4-Tr	imethylpentane	e (1) - Wat	er (2)	System

Reference	T/K	Solubility	Method
Polak and Lu (ref l)	273,298	mutual	GLC, Karl Fischer
Price (ref 2)	298	(l) in (2)	GLC
Krzyzanɔwska and Szeliga (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,3,4-TRIMETHYLPENTANE (1) IN WATER (2)

All the available data on the solubility of 2,3,4-trimethylpentane in water are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 3) which does not appear to be independent of that of Price (ref 2) and has thus been excluded from consideration.

At 298K, the datum of Polak and Lu (ref 1) is much higher than that reported by Price (ref 2), as for many other hydrocarbon systems investigated by these authors. In the absence of other independent studies it is not possible to prefer either datum.

TABLE		Tentative						of
2	<u>,3,</u> 4	4-Trimethylp	pentane	(1)	in	Water	(2)	

<i>Т/</i> К	Solubilit	y values	
	Reported values 10 ⁴ g(1)/100g sln	"Best" values $(\pm \sigma_n)^a$ 10 ⁴ g(1)/100g sln 10	x1
273	2.34 (ref 1)	2.3	
298	2.30 (ref 1), 1.36 (ref 2)	1.8 ± 0.5	

a Obtained by simple averaging, σ_n has no statistical significance.

(continued next page)

COMPONENTS :	EVALUATOR:
 (1) 2,3,4-Trimethylpentane; C₈H₁₈ [565-75-3] (2) Water; H₂O; [7732-18-5] 	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

2. THE SOLUBILITY OF WATER (2) IN 2,3,4-TRIMETHYLPENTANE (1)

As only one study of the solubility of water in 2,3,4-trimethylpentane has been reported (ref 1) no Critical Evaluation is possible. The interested user is referred to the appropriate Data Sheet for experimental values. However, it may be noted that the solubility of water in other hydrocarbons reported by Polak and Lu (ref 1) are normally reliable.

REFERENCES

- 1. Polak, J.; Lu, B.C-Y. Can. J. Chem. <u>1973</u>, 51, 4018-23.
- 2. Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44.
- 3. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.

ORIGINAL MEASUREMENTS:
Polak, J.; Lu, B.C-Y. Can. J. Chem. <u>1973</u> , 51, 4018-23.
PREPARED BY: M.C. Haulait-Pirson
nethylpentane in water sln x_1 (compiler)
$\frac{1}{2} \qquad \frac{1}{3.69 \times 10^{-7}}$ 3.62 × 10 ⁻⁷
2,3,4-trimethylpentane
sln x ₂ (compiler)
1.27×10^{-4} 4.69 x 10^{-4}
INFORMATION ·
<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean) REFERENCES:</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,3,4-Trimethylpentane; C ₈ H ₁₈ ; [565-75-3]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,3,4-trimethylpent	ane in water at 25°C and
at system pressure was reported to be	1.36 mg(l)/kg(2). The
corresponding mass percent and mole f	raction, x,, calculated
by the compiler are 1.36 x 10^{-4} g(1)/	

NFORMATION
NFORMATION SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 0.03 mg(1)/kg(2) REFERENCES:
Et

(1) 2,3,4-Trimethylpentane; $C_{gH_{18}}$; [565-75-3]Krzyzanowska, T.; Szeliga, J. Nafta (Katowice), <u>1978</u> , 12, 413-7(2) Water; H ₂ O; [7732-18-5]Nafta (Katowice), <u>1978</u> , 12, 413-7(2) Water; H ₂ O; [7732-18-5]Nafta (Katowice), <u>1978</u> , 12, 413-7(2) Water; H ₂ O; [7732-18-5]N.C. Haulait-Pirson EXPERIMENTAL VALUES: N.C. Haulait-PirsonThe solubility of 2,3,4-trimethylpentane in water at 25°C was reported to be 1.36 mg(1)/kg(2).N.C. Haulait-PirsonThe corresponding mass percent and mole fraction, x_1 , calculated by compiler are 1.36 x 10 ⁻⁴ g(1)/100 g sln and 2.14 x 10 ⁻⁷ .Editor's Note: Based on the results for this and other hydrocarbon-wate systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). METHOD/AFPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted tarted solutions of heptane in (2)SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. (3) not specified. (4) not specified. (2) not specified. (2) not specified. (3) not specified. (4) not specified. (2) not specified. (3) not specified. (4) not specified. (5) not specified. (6)		ADTATNAT NO ACTIDENTING.
Tafta (Xatowice), 1978, 12, 413-7(2) Water; H20; [7732-18-5]Nafta (Xatowice), 1978, 12, 413-7(2) Water; H20; [7732-18-5]Nafta (Xatowice), 1978, 12, 413-7(2) Water; H20; [7732-18-5]N.C. Haulait-PirsonVARIABLES:N.C. Haulait-PirsonExperimental values:N.C. Haulait-PirsonExperimental values:N.C. Haulait-PirsonExperimental values:N.C. Haulait-PirsonExperimental values:N.C. Haulait-PirsonExperimental values:N.C. Haulait-PirsonEditor's Note: Based on the results for this and other hydrocarbon-wate:systems, uncertainity exists about whether the datum compiled here isindependent of that of Price for the same system (see previous page).METHOD/APPARATUS/PROCEDURE:The saturated solutions of (1) in(2) were prepared in two ways.First, 200 LL of (1) was injectedint 20 mL of (2) and thermostattedint 02 mL of (2) and thermostattedint 02 was measured by glc. APerkin-Elmer model F-11 gas chromat-Oraph equipped with a 100-150 methForasil column (70°C) and a flameionization detector was used.soly. 0.05 mg(1)/kg(2) (standardwere used as standard solutions.	COMPONENTS:	ORIGINAL MEASUREMENTS:
(2) Water, H ₂ O; [7732-18-5] VARIABLES: One temperature: 25°C M.C. Haulait-Pirson EXPERIMENTAL VALUES: The solubility of 2,3,4-trimethylpentane in water at 25°C was reported to be 1.36 mg(1)/kg(2). The corresponding mass percent and mole fraction, x ₁ , calculated by compiler are 1.36 x 10 ⁻⁴ g(1)/100 g sln and 2.14 x 10 ⁻⁷ . Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). AUXILIARY INFORMATION NETHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) ware prepared in two ways. First, 200 LL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model P-11 gas chromator graph equipped with a 100-150 mesh Forasil column (70°C) and a flame in (2) were used as standard solutions.	0 10	
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The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. (1) not specified. (2) not specified. (2) not specified. (3) not specified. (2) not specified. (3) not specified. (3) not specified. (4) not specified. (5) not specified. (5) not specified. (6) not specified. (7) not spec		
 (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. 		
<pre>First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.</pre> (2) not specified. (3) not specified. (4) not specified. (4) not specified. (5) not specified. (5) not specified. (6) not specified. (7)		(1) not specified.
at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. ESTIMATED ERROR:	First, 200 µL of (1) was injected	(2) not specified.
at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. ESTIMATED ERROR: soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations		
<pre>time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. ESTIMATED ERROR: Soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations</pre>		
<pre>(1) in (2) was measured by glc. A Perkin-Elmer model F-ll gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.</pre> ESTIMATED ERROR: Soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations	time required to obtain equilibrium	
Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. ESTIMATED ERROR: soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations		
Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions. ESTIMATED ERROR: soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations	Perkin-Elmer model F-11 gas chromat-	
urated solutions of heptane in (2) were used as standard solutions. deviation from 7-9 determinations	Porasil column (70°C) and a flame	ESTIMATED ERROR:
were used as standard solutions. deviation from 7-9 determinations		solv. 0.05 mg(1)/kg(2) (standard
REFERENCES :		deviation from 7-9 determinations).
		REFERENCES :
1		
•		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylhexane; C ₈ H ₁₈ ; [584-94-1]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.
VARIABLES:	PREPARED BY:
One temperature: not specified	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,3-dimethylhexane 0.0002 mL(1)/L(2).	in water was reported to be
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The procedure is described in ref 1.	not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :
	 Baker, E.G. Am, Chem. Soc., Div. Petrol. Chem., Preprints 1958, 3, N°4, C61.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylhexane; C ₈ H ₁₈ ; [589-43-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson

	Solubility of water in 2,4-dimethylhexane	
t/°C	g(2)/100 g sln	$\frac{10^4 x_2}{2}$ (compiler)
10	0.0053	3.36
20	0.0098	6.21
30	0.0180	11.41

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR: not specified.</pre>	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methylheptane; C₈H₁₈; [589-81-1] (2) Water; H₂O; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

The solubility of 3-methylheptane in water at 25°C and at system pressure was reported to be 0.792 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 7.92 x 10⁻⁵ g(l)/100 g sln and 1.25 x 10⁻⁷.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame iOnization detectors. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 0.028 mg(1)/kg(2) REFERENCES:</pre>		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylheptane; C ₈ H ₁₈ ;	Krzyzanowska, T.; Szeliga, J.
[589-81-1]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

The solubility of 3-methylheptane in water at 25°C was reported to be 0.792 mg(l)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 7.92 x 10^{-5} g(l)/100 g sln and 1.25 x 10^{-7} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	<pre>(1) not specified. (2) not specified. ESTIMATED ERROR:</pre>		
	soly. 0.04 mg(l)/kg(2) (standard deviation from 7-9 determinations).		
	REFERENCES :		

*	COMPONENTS:	EVALUATOR:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] and Physical Sciences, Murdoch	0 10	University, Perth, W.A., Australia.

CRITICAL EVALUATION:

Quantitative solubility data for the n-octane (1) - water (2) system have been reported in the publications listed in Table 1.

	T/K	Solubility	Method
Fühner (ref 1)	289	(1) in (2)	titration
Black et al. (ref 2)	293	(2) in (1)	radiotracer
Baker (ref 3)	unspecified	(1) in (2)	radiotracer
Englin (ref 4)	283-303	(2) in (1)	analytical
McAuliffe (ref 5)	298	(l) in (2)	GLC
Nelson and De Ligny (ref 6)	278-318	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 9)	298	(1) in (2)	GLC
Polak and Lu (ref 10)	273,298	mutual	GLC, Karl Fischer
Budantseva <i>et al</i> . (ref 11)	293	mutual	unspecified
Price (ref 12)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 13)	298	(1) in (2)	GLC
Skripka (ref 14)	498-538 ^a	(2) in (l)	unspecified
Jonsson et al. (ref 15)	288-308	(l) in (2)	partition coefficient
Heidman <i>et al</i> . (ref 16)	311 - 539 ^a	mutual	synthetic

TABLE 1: Quantitative Solubility Studies of theOctane (1) - Water (2) System

a High pressure data

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition critical phenomena have been investigated by Roof (ref 8). These are considered along with solubility data at high pressures in Section 3 below.

For convenience further discussion of this system will be in three parts.

1. THE SOLUBILITY OF OCTANE (1) IN WATER (2)

Agreement amongst the independent determinations of the solubility of octane in water is not particularly good and no data have been Recommended.

At 298K the value reported by Price (ref 11) is substantially lower than all other studies (ref 5,9,10,15) and has been rejected. At higher temp-(continued next page

COMPONENTS:	EVALUATOR:
(2) Mator: H_{0} (7722-18-5)	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

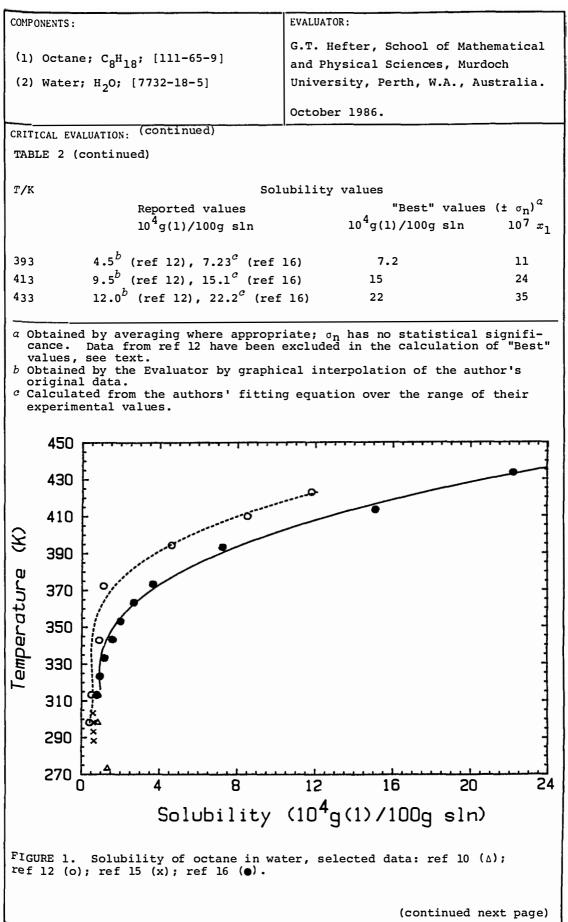
eratures the values of Price (ref 12) are also considerably lower than those of Heidman *et al.* (ref 16). In the absence of confirmatory studies, it is not reasonable to reject Price's data outright but they have not been used in the calculation of "Best" values. Application of the van't Hoff equation to both data sets gives values of $\Delta H_{sln} = -3.3$ (ref 12) and +13.3 (ref 16) kJ mol⁻¹ and $\Delta C_{p,sln} = 568$ (ref 12) and 284 (ref 16) J K⁻¹ mol⁻¹. Neither set of values are close to those reported for related systems although those of Heidman *et al.* are somewhat more reasonable.

At other temperatures the data of Fühner (ref 1), Nelson and De Ligny (ref 6), and Budantseva *et al.* (ref 11) are markedly higher than all other studies and are therefore rejected. All the remaining data are summarized in Table 2 and selected data are plotted in Figure 1.

It is interesting to note that the averaged "Best" value at 298K is very close to the value which would be predicted by an extrapolation of the lower n-alkane solubilities.

T/K	Solubility values		
	Reported values	"Best" value	es ($\pm \sigma_n$) ^a
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ x ₁
273	1.35 (ref 10)	1.4	2.2
293	0.628 (ref 15)	0.63	0.99
298	0.66 (ref 5), 0.70 (ref 9), 0.85 (ref 10), 0.615 (ref 15)	0.71 ± 0.09	1.1
303	0.46 ^b (ref 12), 0.612 (ref 15)	0.61	0.96
313	0.52 ^b (ref 12), 0.80 ^c (ref 16)	0.8	1.3
323	0.61 ^b (ref 12), 0.96 ^c (ref 16)	1.0	1.6
333	0.74 b (ref 12), 1.2 c (ref 16)	1.2	1.9
343	0.91 b (ref 12), 1.5 c (ref 16)	1.5	2.4
353	1.0^{b} (ref 12), 1.99 c (ref 16)	2.0	3.2
363	1.1^{b} (ref 12), 2.67 ^c (ref 16)	2.7	4.3
373	1.2^{b} (ref 12), 3.66 ^c (ref 16)	3.7	5.8

TABLE 2: Tentative Values of the Solubility of Octane (1) in Water (2)



COMPONENTS :	EVALUATOR:
(2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

2. THE SOLUBILITY OF WATER (2) IN OCTANE (1)

Only limited data are available for the solubility of water in *n*-octane and agreement amongst independent determinations is only fair. The datum of Black *et al.* (ref 2) is much higher than all other values and is therefore rejected. The remaining data are collected in Table 3 and plotted in Figure 2.

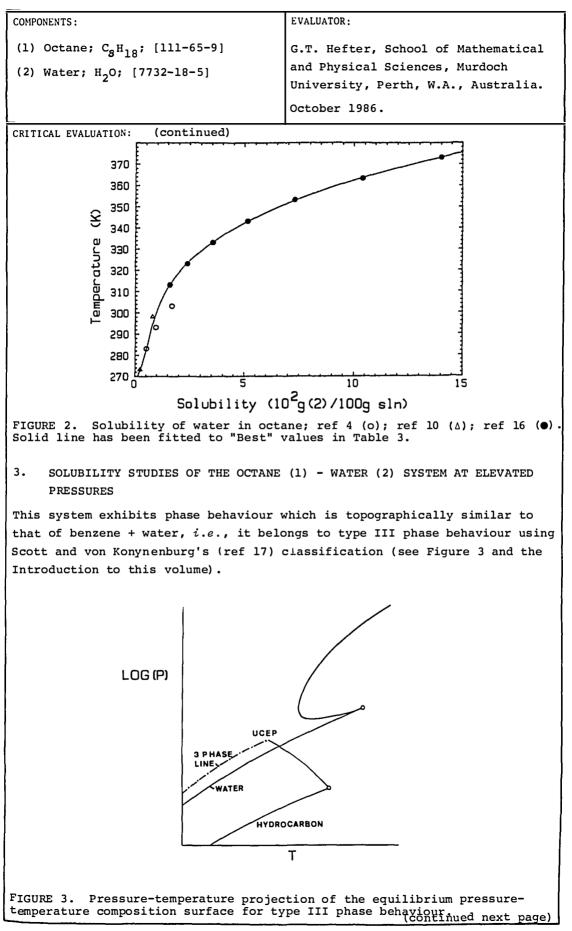
TABLE 3:Tentative Values of the Solubility ofWater (2) in Octane (1)

T/K	Solubility values		
	Reported values	"Best" values (:	
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	10 ⁴ x ₂
273	0.23 (ref 9)	0.2	1
283	0.51 (ref 4)	0.5	3
29 3	0.95 (ref 4), 0.68 (ref 10)	0.8 ± 0.1	5
298	1.26 ^b (ref 4), 0.79 (ref 9)	1.0 ± 0.2	6
303	1.68 (ref 4)	1.7	11
313	1.58 c (ref 14)	1.6	10
323	2.40^{c} (ref 14)	2.4	15
333	3.54^{c} (ref 14)	3.5	22
343	5.14 c (ref 14)	5.1	32
353	7.30^{c} (ref 14)	7.3	46
363	10.2^{c} (ref 14)	10	63
373	14.0 [°] (ref 14)	14	89

a Obtained by averaging where appropriate; σ_n has no statistical significance.

b Obtained by graphical interpolation (Evaluator) of authors' original data. c Calculated (Evaluator) from fitting equation given by authors, over the range of their experimental values.

(continued next page)



COMPONENTS:	EVALUATOR:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

Quantitative solubility data on the octane - water system at elevated pressures have been reported in the studies listed in Table 4.

TABLE 4. Solubility Studies of the Octane (1) - Water (2) System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Roof (ref 8)	_a	_ ^a	_a
Price (ref 12)	_b	298-423	(1) in (2)
Skripka (ref 14)	3.5-78.5	498-538	(2) in (1)
Heidman <i>et al</i> . (ref 16)	0.01-8.9 ^b	311-539	mutual

a Critical point of unspecified composition. b Along the three-phase line.

As can be seen from Table 4 data have not generally been obtained under comparable conditions, making Critical Evaluation difficult. However, it may be noted that the solubility of 9.95 g(2)/100g sln of water in octane at 7.4 MPa and 538.2 K reported by Skripka (ref 14) differs markedly from the value of 14.9 g(2)/100g sln reported at 7.41 MPa and 539.1 K by Heidman *et al.* (ref 16). Further studies are necessary before any preference can be expressed for either data set. Previous mention (Section 1 above) has already been made of the fact that the solubilities of octane in water reported by Heidman *et al.* (ref 16) are much higher than those of Price (ref 12).

On the other hand the properties of the critical end point (Figure 3) reported by Roof: 7.41 MPa and 540.4 K, are in good agreement with those reported by Heidman *et al.* (ref 16): 7.41 MPa and 539.1 K.

COMPO	DNENTS:	EVALUATOR:	
(1)	Octane; C ₈ H ₁₈ ; [111-65-9]	G.T. Hefter, School of Mathematical	
	0 20	and Physical Sciences, Murdoch	
(2)	Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.	
		October 1986.	
CRITI	CAL EVALUATION: (continued)		
REFI	ERENCES		
1.	Fühner, H. Chem. Ber. <u>1924</u> , 57	, 510-5.	
2.	Black, C.; Joris, G.G.; Taylor, H	H.S. J. Chem. Phys. <u>1948</u> , 16, 537-48.	
з.	Baker, E.G. Geochim. Cosmochim.	Acta <u>1960</u> , <i>19</i> , 309-17.	
4.	Englin, B.A., Plate, A.F.; Tugolu Tekhnol. Topl. Masel <u>1965</u> , 10, 4		
5.	McAuliffe, C. J. Phys. Chem. 19	9 <u>66</u> , 70, 1267-75.	
6.	Nelson, H.D.; De Ligny, C.L. <i>Rec. Trav. Chim. Pays-Bas</i> <u>1968</u> , 87, 528-44.		
7.*			
8.	Roof, J.G. J. Chem. Eng. Data	<u>970, 15, 301-3.</u>	
9.	Krasnoshchekova, P.Y.; Gubergrits 885-7.	5, M.Y. Neftekhimiya <u>1973</u> , 13,	
10.	Polak, J.; Lu, B.C-Y. Can. J. Ch	nem. <u>1973, 51, 4018-23.</u>	
11.	. Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. <i>Zh. Fiz. Khim.</i> <u>1976</u> , 50, 1344, Deposited doc. 1976, VINITI 437-76.		
12.			
13.			
14.			
15.	Jonsson, J.A.; Vejrosta, J.; Nova 279-86.	uk, J. Fluid Phase Equil. <u>1982</u> , 9,	
16.	Heidman, J.L.; Tsonopoulos, C.; E <u>1985</u> , <i>31</i> , 376-84.	brady, C.J.; Wilson, G.M. A.I.Ch.E.J.	
17.	Scott, R.L.; van Konynenburg, P.H. <u>1980</u> , <i>A298</i> , 495.	. Phil. Trans. Roy. Soc. London	
ACKNOWLEDGEMENT			
The	The Evaluator thanks Dr Brian Clare for the graphics.		
*NOTE ADDED IN PROOF			
Delete ref 7.			

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Fühner, H.
(2) Water; H ₂ O; [7732-18-5]	Ber. Dtsh. Chem. Ges. <u>1924</u> , 57, 510-5.
VARIABLES:	PREPARED BY:
	N.C. Newloit Dimen
One temperature: 16°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of octane in water at	16°C was reported to be
0.002 mL(1)/100 mL sln or 0.0014 g(1)	/100 g sln.
The corresponding mole fraction, x_1 ,	calculated by the compiler
is 0.22 x 10 ⁻⁵ .	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The stonewed reserving culinder	(1) source not specified; commer-
In a stoppered measuring cylinder pipetted volumes or weighed amounts	cial grade; used as received.
of (1) were added with shaking to 50, 100 or 1000 cm^3 of (2) until a	(2) not specified.
completely clear solution was	
obtained at the experimental tem- perature.	
	ESTIMATED ERROR:
	not specified.
	-
	REFERENCES:
	1

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Black, C.; Joris, G.G.; Taylor, H.S.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Phys. <u>1948</u> , 16, 537-43.
_	
VARIABLES:	PREPARED BY:
One temperature: 20°C	M.C. Haulait-Pirson
Experimental values:	
The solubility of water in octane at saturation pressure of 1 atm was report The corresponding mass percent and mo by the compiler are 0.0142 g(2)/100 g	prted to be 0.0142 g(2)/100 g(1). Dle fraction, x_2 , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method described in ref 1 in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.	project; purity not specified; used as received.
	ESTIMATED ERROR:
	soly. a few percent (type of error not specified).
	REFERENCES: 1. Joris, G.G.; Taylor, H.S. J. Chem. Phys. <u>1948</u> , 16, 45.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1960</u> , 19, 309-17.
VARIABLES:	PREPARED BY:
One temperature: not specified.	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	•
The solubility of octane in water was 0.09 x 10 ⁻⁶ mL(1)/mL(2).	reported to be
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined after ultrafiltration using the procedure described in ref 1.	not specified.
	not specified.
	REFERENCES: 1. Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprint <u>1958</u> , 3, N°4, C61.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson

Solubility	of	water	in	octane
------------	----	-------	----	--------

t/°C	g(2)/100 g sln	$\frac{10^4 x_2}{2}$ (compiler)
10	0.0051	3.24
20	0.0095	6.03
30	0.0168	10.65

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, cal- cium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) not specified.(2) not specified.	
	ESTIMATED ERROR: not specified.	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of octane in water at be 0.66 mg (1)/kg sln. The corresponding mole fraction, x_1 , is 1.04 x 10 ⁻⁷ . The same value is also reported in re	calculated by the compiler,
A 11 V T T A D V	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph. A hydrogen-flame ionization detector	<pre>(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.06 mg (1)/kg sln (standard</pre>
was used. Many details are given in the paper.	deviation from mean)
	REFERENCES :
	 McAuliffe, C. Nature (London) <u>1963</u>, 200, 1092. McAuliffe, C. Am. Chem. Soc., Div. Petrol. Chem. <u>1964</u>, 9, 275.

38_109	147
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Nelson, H.D.; De Ligny, C.L.
(2) Water, H ₂ O; [7732-18-5]	Rec. Trav. Chim. Pays-Bas <u>1968</u> , 87, 528 - 44.
VARIABLES:	PREPARED BY:
Temperature: 5-45°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of oct	cane in water
$t/^{\circ}C$ $10^{7}x$	mg(l)/kg sln (compiler)
5.0 2.6 ± (0.6 1.65
15.0 1.4 ± 0	
45.0 2.9 ± (0.6 1.84
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation vessel is drawn in the original paper. (2) was satu- rated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chro- matographic conditions are described in the paper.	more. ESTIMATED ERROR: soly.: error given above (standard

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of octane in water at $x_1 = 1.0 \times 10^{-7}$. The corresponding mass percent calculation 7.0 $\times 10^{-5}$ g(1)/100 g sln.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air,	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled.</pre>
and the (1)-saturated air was	ESTIMATED ERROR:
analyzed by glc.	not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	ORIGINAL IERBORCIENTS.
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Polak, J.; Lu, B.C-Y.
(2) Water; H ₂ O; [7732-18-5]	Can. J. Chem. <u>1973</u> , 51, 4018-23.
VARIABLES :	
	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·
Solubility of oc	tane in water
t/°C mg(l)/kg	sln x ₁ (compiler)
	c 2.13 x 10 ⁻⁷
25 ^b 0.85	_
Solubility of wa	ter in octane
t/°C mg(2)/kg	$sln = \pi_2$ (compiler)
0 ^a 23 ^d	1.46×10^{-4}
23 ⁻ 23 ⁻ 23 ⁻	1.46×10^{-4} 5.01 × 10 ⁻⁴
	5.01 × 10
^{a-e} See "Estimated Error"	
See Estimated Error	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was	(1) Phillips Petroleum Co.; pure
determined by gas chromatography. The solubility of (2) in (1) was	grade reagent (99%+); shaken three times with distilled
determined by Karl Fischer titra-	water.
tion. 50 mL of (1) together with 50 mL of (2) were placed in a 125	(2) distilled.
mL Hypovial closed with a Teflon coated rubber septum and placed in	
a constant-temperature water bath. The system was stirred magnetical-	
ly for 24 hr or was kept in the	
bath without stirring for at least 7 days before samples were taken	ESTIMATED ERROR:
for analysis. Details of the analysis are given in the paper.	temp. a) ± 0.02°C; b) ± 0.01°C soly. c) ± 4%; d) ± 4.7%;
	e) ± 3.1% (mean)
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]	 Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. <i>Zh. Fiz. Khim.</i> <u>1976</u>, 50, 1344. <i>Deposited doc.</i> <u>1976</u>, VINITI 437-76. 	
VARIABLES:	PREPARED BY:	
One temperature: 20°C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of octane in water at $x_1 \approx 2 \times 10^{-7}$. The corresponding mass percent calcul		
about 0.0001 g(1)/100 g sln.		
The solubility of water in octane at $x_2 = 4.3 \times 10^{-4}$.	20°C was reported to be	
The corresponding mass percent calculated by the compiler is 0.007 g(2)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
TETROD ATTACATOS / TROCEDORE .	SOURCE AND FURTH OF PATERIALS.	
Nothing specified in the paper.	(1) not specified.	
	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
VARIABLES:	PREPARED BY:
Temperature: 25-149.5°C	F. Kapuku

Solubility	of	octane	in	water	at	system	pressure
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t/°C	mg(l)/kg(2)	g(l)/l00 g sln (compiler)	$10^{7}x_{1}$ (compiler)
25.0	0.431 ± 0.012	0.0000431	0.680
40.1	0.524 ± 0.021	0.0000524	0.826
69.7	0.907 ± 0.042	0.0000907	1.43
99.1	1.12 ± 0.07	0.000112	1.77
121.3	4.62 ± 0.22	0.000462	7.29
136.6	8.52 ± 0.34	0.000852	13.4
149.5	11.80 ± 0.7	0.00118	18.6

AUXILIARY	INFORMATION
NUVITIUVI	THEORETION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed	 (1) Phillips Petroleum Company; 99+%. (2) distilled.
the bottom of the cylinder and al- lowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given	ESTIMATED ERROR: temp. ± 1°C soly. range of values given above
in the paper.	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water, H ₂ O; [7732-18-5]	 Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u>, 61, 139-51. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u>, 47, 1035.
VARIABLES:	PREPARED BY:
Temperature: 225-265°C Pressure: 3.5-78.5 MPa	A. Maczynski

Solubil	lity of water in	n octane .	
$p/kg cm^{-2}$	p/MPa (compiler)	<i>x</i> ²	g(2)/100 g sln (compiler)
36 100 200 300 400 500 600 700 800	3.5 9.8 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.166 0.137 0.109 0.098 0.091 0.088 0.084 0.080 0.075	3.04 2.44 1.89 1.68 1.55 1.50 1.42 1.35 1.26
50 100 200 300 400 500 600 700 800	4.9 9.8 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.216 0.193 0.164 0.149 0.140 0.132 0.126 0.122 0.117	4.16 3.63 3.00 2.69 2.50 2.34 2.22 2.14 2.05 (continued)
		(4 TTO)	(continued)
rimental technique d in ref 1. No det	was (1) ails	source not spe reagent grade; specified; use	cified, chemical
	1. 5	Sultanov, R.G.; Namiot, A.Yu.	
	<pre></pre>	p /kg cm ⁻² p /MPa (compiler) 36 3.5 100 9.8 200 19.6 300 29.4 400 39.2 500 49.0 600 58.8 700 68.6 800 78.5 50 4.9 100 9.8 200 19.6 300 29.4 400 39.2 500 4.9 100 9.8 200 19.6 300 29.4 400 39.2 500 49.0 600 58.8 700 68.6 800 78.5 SOURC In the paper. (1) In the paper. (2) ESTIN not REFEE 1. S 1. S 1. S	36 3.5 0.166 100 9.8 0.137 200 19.6 0.109 300 29.4 0.098 400 39.2 0.091 500 49.0 0.088 600 58.8 0.084 700 68.6 0.080 800 78.5 0.075 50 4.9 0.216 100 9.8 0.193 200 19.6 0.164 300 29.4 0.149 400 39.2 0.140 500 4.9 0.126 100 9.8 0.123 600 58.8 0.122 600 58.8 0.122 800 78.5 0.117

(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water; H ₂ O; [7732-18-5]		Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u> , 61, 139-51.		
		Sultanov, R.G.; S Zh. Fiz. Khim. <u>19</u>		
t/°C	p/kg cm ⁻²	p/MPa (compiler)	<i>x</i> ²	g(2)/100 g sln (compiler)
265	75 100 200 300 400 500 600 700 800	7.4 9.8 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.412 0.350 0.254 0.224 0.207 0.194 0.183 0.172 0.163	9.95 7.83 5.10 4.35 3.95 3.66 3.41 3.19 2.98

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of octane in water at	25°C was reported
	25 C was reported
to be 0.431 mg(1)/kg(2).	
The corresponding mass percent and m	Ĩ
by compiler are 4.31 x 10^{-5} g(1)/100	g sln and 6.80 x 10 $^{\circ}$.
Editor's Note: Based on the results	for this and other hydrocarbon-water
systems, uncertainity exists about w	hether the datum compiled here is
independent of that of Price for the	same system.
	INFORMATION
	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:	
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.
First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted	(2) not specified.
at 25°C. Second, the mixture of (1) and (2) as above was thermostatted	
at 70°C and then cooled to 25°C. The time required to obtain equilibrium	e
was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-ll gas chromat-	
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	
l dan daa daa daa daa daa daa daa daa daa	ESTIMATED ERROR:
ionization detector was used. Sat- urated solutions of heptane in (2)	
ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	ESTIMATED ERROR: soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations).
urated solutions of heptane in (2)	<pre>soly. 0.02 mg(1)/kg(2) (standard</pre>
urated solutions of heptane in (2)	soly. 0.02 mg(l)/kg(2) (standard deviation from 7-9 determinations).
urated solutions of heptane in (2)	soly. 0.02 mg(l)/kg(2) (standard deviation from 7-9 determinations).
urated solutions of heptane in (2)	soly. 0.02 mg(l)/kg(2) (standard deviation from 7-9 determinations).

COMPONENTS :	ORIGINAL MEASUREMENTS:		
	OKIOINAL ILABORDILINIDI		
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Jonsson, J.A.; Vejrosta, J.; Novak, J.		
(2) Water; H ₂ O; [7732-18-5]	Fluid Phase Fruit 1092 0 270-96		
	Fluid Phase Equil. <u>1982</u> , 9, 279-86.		
VARIABLES:	PREPARED BY:		
Temperature: 15-35°C	G.T. Hefter		
EXPERIMENTAL VALUES:			
	octane in water		
t/°C mg(l)/kg sln	10 ⁵ g(1)/100g sln 10 ⁷ x1 (compiler) (compiler)		
15 0.653	6.53 1.03		
20 0.628	6.28 0.99		
	6.15 0.97 6.12 0.96		
30 0.612 35 0.620	6.20 0.98		
35 0.620	6.20 0.96		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapour concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analysed by gas chromatography. The method and apparatus are described in detail in ref 1.	 (1) Fluka, > 99.8%, used as received. (2) Not specified. 		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		
	<pre>1. Vejrosta, J.; Novak, J.; Jonsson, J.A. Fluid Phase Equil. <u>1982</u>, 8, 25-35.</pre>		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Water, H ₂ O; [7732-18-5]	Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. A. I. Ch. E. J. <u>1985</u> , <i>31</i> , 376-84.
VARIABLES: Temperature: 311-553 K Pressure: 0.01-7.4 MPa	PREPARED BY: G.T. Hefter

	Solubility of	octane in water	
T/K	p /MPa	10 ⁵ x ₁	<pre>10² g(l)/100 g sln (compiler)</pre>
310.9	0.0103 ^a	0.012	0.0076
366.5	0.117 ^a	0.048	0.030
422.0	0.655	0.38	0.24
479.5	2.51	4.0	2.5
536.1	7.03	35	22
552.8	8.86	60 ^{<i>b</i>}	38

a Estimated by the authors from pure component data

b Above three-phase equilibrium point.

(continued)

AUXILIARY	INFORMATION
METHOD /APPARATUS /PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observ- ation. This aspect of the procedure is discussed in detail in the paper.	purity ≥99.9 mol %, checked by gas chromatography.
	<pre>ESTIMATED ERROR: soly. ± 5%, relative precision of replicate analyses. temp. not stated. press. ± 1%; type of error not stated. REFERENCES: 1. Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. <u>1983</u>, 29, 990-9.</pre>

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(1) Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
(2) Water, H<sub>2</sub>O; [7732-18-5]
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(continued)

Solubility of water in octane

<i>т</i> / к	р /МРа	10 ² x ₂	g(2)/100 g sln (compiler)
310.9	0.0103 ^{<i>a</i>}	0.100	0.0158
366.5	0.117	0.62	0.098
422.0	0.655	3.94	0.622
477.6	_ <i>b</i>	12.6	2.22
533.1	_ <i>b</i>	38.7	9.05
539.1 [°]	7.41	52.7 [°]	14.9
550.4 ^d	-	54.9 ^d	16.1

a Estimated by the authors from pure component data.

b Not specified.

c Three phase critical point.

d Above three phase critical point.

The three phase critical point was reported to be 539.1 \pm 0.6 K, 7.37 \pm 0.04 MPa and $x_1 = 4.61 \times 10^{-4}$ (0.292 g(1)/100 g sln, compiler).

The authors also report equations which fit their own and literature data over the range 273-539 K, viz.

 $\ln x_1 = -343.1497 + 13862.49/T + 49.24609 \ln T$ $\ln x_2 = -0.66037 - 7.1130 (T_r^{-1} - 1) - 0.67885 (1 - T_r)^{1/3}$ $- 1.43381 (1 - T_r)$

where $T_{n} = T/539.1$

COMPONENTS:	EVALUATOR:
(1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of octane (1) in seawater (2) has been reported in two works:

Authors	Method	т/к	Salinity g salts/kg sln	g(l)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	2.5×10^{-4}
Freegarde <i>et al</i> . (ref 2)	GLC	?	?	1×10^{-4}

Because temperature and salinity are not specified, the data of Freegarde *et al.* are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of octane in pure water at 298 K.

SOLUBILITY	OF	OCTANE	(1)	IN	SEAWATER	(2)
DOUBTFUL VALUE						

т/к	g salts/kg sln	g(l)100 g sln
298	6	2.5×10^{-4}

REFERENCES

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u>, 13, 885-8.
- Freegarde, M.; Hatchard, C.G.; Parker, C.A. Lab. Pract. <u>1971</u>, 20, 35-40.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Freegarde, M.; Hatchard, C.G.; Parker, C.A.
<pre>(2) Seawater (composition not specified)</pre>	Lab Pract. <u>1971</u> , 20, 35-40.
VARIABLES:	PREPARED BY:
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of octane was reported	to be 1.0 mg/L. The
corresponding mass percent and mole f	raction, x_1 , calculated
by the compilers are 1.0 x 10^{-4} g(1)/	100 g sln and 1.6 x 10^{-7} ,
assuming a solution density of 1.02 k	g/L.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
None given except that analysis was done using gas chromatography.	not given.
· ·	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C ₈ H ₁₈ ; [111-65-9]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Seawater	Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885-8.
	,,,
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of octane in seawater	was reported to be
$2.5 \times 10^{-4} \text{ g(1)}/100 \text{ g sln. and the c}$	orresponding mole fraction,
$x_1 = 4.0 \times 10^{-7}$.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared	(1) "chemically pure"
by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs.	(2) distilled water plus salt
in a flask placed in a temperature controlled bath. A sample of solu-	mixture.
tion was then transferred to a closed flask with head space volume	
equal to solution volume. Hydro- carbon concentration in the head	
space was determined by gas chroma- tography and the corresponding solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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2.

(1) Indan; C ₉ H ₁₀ ; [496-11-7] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.
]	February 1986.

CRITICAL EVALUATION:

Quantitative solubility studies for indan (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1.	Quantitative Solubility Studies of	
	Indan (1) in Water (2)	

Reference	<i>Т/</i> К	Method
Price (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data in these publications are compiled in the Data Sheets immediately following this evaluation. No data have been reported on the solubility of water in indan.

The data of Price (ref 1) and Mackay and Shiu (ref 2) are in good agreement (Table 2) although the relative uncertainty (\pm 10%) is too large for the mean to be Recommended given the relatively high solubility. Further studies are required.

TABLE 2: Tentative Value of the Solubility ofIndan (1) in Water (2)

<i>т/</i> к	Solubility value					
		Reported va		"Best"	value (±ơ _n)	_
	1	.0 ² g(1)/100g	g sln	10 ² g(1)/100	g sln	10 ⁵ <i>x</i> 1
298	0.889	(ref 1), 1.	.091 (ref 2)	1.0 ± 0	.1	1.5
REFERENC	ES					
l. Pri	ce, L.C.	Am. Assoc.	Petrol. Geol.	Bull. <u>1976</u> , 6	0, 213-44.	

Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Indan; C ₉ H ₁₀ ; [496-11-7]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES :	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of indam in water at 25°C and at system pressure was reported to be 88.9 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00889 g(l)/ 100 g sln and 1.35 x 10⁻⁵.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

 Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

```
(2) distilled.
```

ESTIMATED ERROR: temp. ± 1°C soly. ± 2.7 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Indan; C ₉ H ₁₀ ; [496-11-7]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of indan in water at to be 109.1 mg(1) dm ⁻³ sln and $x_1 =$ The corresponding mass percent calcu is 0.01091 g(1)/100 g sln.	1.665×10^{-5} .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>Source AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 1.02 mg(1) dm⁻³ sln (maximum deviation from several determina- tions). REFERENCES:</pre>

COMPONENTS :	EVALUATOR:
[526-73-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.
	December 1986

CRITICAL EVALUATION:

Quantitative solubility data for 1,2,3-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,2,3-trimethylbenzene.

TABLE 1: Quantitative Solubility Studies of1,2,3-Trimethylbenzene (1) in Water (2)

Reference	T/K	Method
Sutton and Calder (ref 1)	298	GLC
Sanemasa <i>et al</i> . (ref 2)	288-318	spectrophotometry

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The available data are summarized in Table 2. At 298K, the only temperature where comparison is possible, the data of Sutton and Calder (ref 1) and Sanemasa *et al.* (ref 2) are in reasonable agreement (Table 2) and their average may be considered as the Tentative solubility.

At other temperatures, only the data of Sanemasa $et \ al$. are available so no Critical Evaluation is possible. Nevertheless, it may be noted that for other hydrocarbons in water the data of Sanemasa $et \ al$. are normally reliable.

TABLE 2: Tentative Values of the Solubility of1,2,3-Trimethylbenzene (1) in Water (2)

Т/К	Solubil	ity values	
	Reported values	"Best" values (
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	10 ⁶ x ₁
288	5.99 (ref 2)	6.0	9.0
298	7.52 (ref 1), 6.27 (ref 2)	6.9 ± 0.5	10
308	7.22 (ref 2)	7.2	11
318	8.52 (ref 2)	8.5	13

a Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. December 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
- Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

166	38_123
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8] (2) Water; H₂0; [7732-18-5]</pre>	Sutton, C.; Calder J.A. J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of 1,2,3-trimethylben: to be 75.2 mg(1)/kg(2). The correspondence x_1 , calculated by the compilers are x_1 . 1.126 x 10 ⁻⁵ .	onding mass percent and mole fraction,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chromatography.	 Aldrich Chemical Co. or Matheson Coleman and Bell purified by distillation through a Vigreaux Column; 94.4% purity determined by gas chromatography. Distilled.
	ESTIMATED ERROR:
	Temp. ±0.1°C Soly. 0.6 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1.2.2- $m_{rimothulbongonos}$ C.H.	Sanemasa, I.; Araki, M.;
<pre>(1) 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8]</pre>	Deguchi, T.; Nagai, H.
(2) Water; H ₂ O; [7732-18-5]	Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054–62.
(2) Waller; n ₂ 0; [//32-16-5]	
VARIABLES:	PREPARED BY:
Temperature: 15-45°C	G.T. Hefter
EXPERIMENTAL VALUES:	
The solubility of 1,2,3-t	rimethylbenzene in water
	IIMethylbenzene in water
$t/^{\circ}$ C 10 ⁴ mol(1)/dm ³ sln	$10^3 g(1)/100 g sln 10^6 x_1$
	(compiler) ^a (compiler) ^a
_ _	
	5 00 0 05
15 4.98 ± 0.19	5.99 8.97
25 5.20 ± 0.32	6.27 9.40
35 5.97 ± 0.41	7.22 10.8
45 7.02 ± 0.19	8.52 12.8
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots	 (1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), no stated purity, used without further purification. (2) Redistilled; no further details given.
were withdrawn into separatory	
funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.	ESTIMATED ERROR: soly. see table, type of error not specified. temp. ± 0.01°C.
	REFERENCES:
	1. Kell, G.S. J. Chem. Eng. Data <u>1975</u> , 20, 97.
	 Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. 1981, 225-8.

(1) 1,2,3-Trimethylbenzene; CgH12; [526-73-8] Sutton, C.; Calder, J.A. (2) Artificial seawater (ref 1) J. Chem. Eng. Data 1975, 20, 320-2. VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln PREPARD BY: M. Kleinschmidt EXPERIMENTAL VALUES: The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, s1 calculated by the compiler are 4.86 x 10 ⁻³ g(1)/100 g sln and 7.47 x 10 ⁻⁶ assuming the artificial seawater composition of ref 1. KETHOD/AFPARATUS/FROCEDURE: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the wapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography. SOURCE AND FURITY OF MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 994% pure. (2) made from doubly distilled water and salts 994% pure. ESTIMATED ERROR: temp. t 0.1°C soly. 0.5 (std. dev.) EFERENCES: 1. Lyman, J.; Fleming, R.H.;	68	38_125
One temperature: 25.0°C M. Kleinschmidt EXPERIMENTAL VALUES: M. Kleinschmidt The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 4.86 x 10 ⁻³ g(1)/100 g sln and 7.47 x 10 ⁻⁶ assuming the artificial seawater composition of ref 1. AUXILLARY INFORMATION METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexaper phase. The saturated solution was extracted schromatography. Source Armo Durity of MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99th pure. (2) made from doubly distilled water and salts 99th pure. (2) made from doubly distilled water and salts 99th pure. ESTIMATED ERROR: temp. ± 0.1°C soly. 0.5 (std. dev.) REFERENCES: 1. Lyman, J.; Fleming, R.H.;	C ₉ H ₁₂ ; [526-73-8]	Sutton, C.; Calder, J.A.
The solubility of 1,2,3-trimethylbenzene in artificial.seawater is reported to be 48.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, s_1 calculated by the compiler are 4.86 x 10 ⁻³ g(1)/100 g sln and 7.47 x 10 ⁻⁶ assuming the artificial seawater composition of ref 1. AUXILIARY INFORMATION METHOD/APPARATUS/FROCEDURE: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography. SOURCE AND FURITY OF MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (2) made from doubly 99+% pure. ESTIMATED ERROR: temp: ± 0.1*C soly. 0.5 (std. dev.) REFERENCES: I. Lyman, J.; Fleming, R.H.;	One temperature: 25.0°C	
<pre>METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.</pre> SOURCE AND FURITY OF MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (3) made from doubly distilled water and salts 99+% pure. (4) made from doubly distilled water and salts 99+% pure. (5) made from doubly distilled water and salts 99+% pure. (6) mater and salts 99+% pure. (7) mater and salts 99+% pure. (8) mater and salts 99+% pure. (9) mater and salts 99+% pure. (9) mater and salts 99+% pure. (9) mater and salts 99+% pure. (1) from either Aldrich Chemical Bell, 99+% pure. (2) mater and salts 99+% pure. (2) mater and salts 99+% pure. (3) mater and salts 99+% pure. (4) mater and salts 99+% pure. (5) mater and salts 99+% pure. (6) mater and salts 99+% pure. (7) mater and salts 99+% pure. (8) mater and salts 99+% pure. (9) mater and salts 90+% pure. (9) mater and 9) ma	The solubility of 1,2,3-trimethylber reported to be 48.6 mg(1)/kg sln. T mole fraction, x_1 calculated by the	The corresponding mass percent and compiler are 4.86 x 10^{-3} g(1)/100 g
 A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography. (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (3) made from doubly distilled water and salts 99+% pure. (4) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (3) made from doubly distilled water and salts 99+% pure. (4) made from doubly distilled water and salts 99+% pure. (5) made from doubly distilled water and salts 99+% pure. (6) made from doubly distilled water and salts 99+% pure. (7) made from doubly distilled water and salts 99+% pure. (8) made from doubly distilled water and salts 99+% pure. (9) made from doubly distilled water and salts 99+% pure. (9) made from doubly distilled water and salts 99+% pure. (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. (3) for the form double distilled water and salts 99+% pure. (4) for the form double distilled water and salts 99+% pure. (5) for the form double distilled water and salts 99+% pure. 	AUXILIARY	INFORMATION
<i>v. Mar. Neb.</i> <u>1740</u> , <i>b</i> , 155.	A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas	 (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. ESTIMATED ERROR: temp. ± 0.1°C soly. 0.5 (std. dev.) REFERENCES:

COMPONENTS:	EVALUATOR:
<pre>(1) 1,2,4-Trimethylbenzene; C₉H₁₂; [95-63-6] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
_	August 1985.

CRITICAL EVALUATION:

Quantitative solubility data for 1,2,4-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of 1,2,4-Trimethylbenzene (1) in Water (2)		
Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Sutton and Calder (ref 2)	298	GLC
Price (ref 3)	298	GLC
Krzyzanowska and Szeliga (ref 4)	298	GLC
Sanemasa <i>et al</i> . (ref 5)	288-318	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data have been reported for the solubility of water in 1,2,4-trimethylbenzene.

All the available data are collected in Table 2 with the exception of that of Krzyzanowska and Szeliga (ref 4) which does not appear to be independent of that of Price (ref 3) and thus has been excluded from consideration. At 298K the only temperature where comparison is possible, the data are in excellent agreement so that the mean can be Recommended, although interestingly the value of Price (ref 3) is somewhat lower than those reported by other workers as for many of the higher hydrocarbons investigated by this author. At other temperatures only the data of Sanemasa *et al.* (ref 5) are available and must thus be regarded as Tentative.

TABLE 2:	Recommended (R) and Tentative Values of the Solubility	
	of 1,2,4-Trimethylbenzene (1) in Water (2)	

T/K	Solubility values		
	Reported values	"Best" values	(±σn) ^a
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	^{"10⁶ x₁}
288	5.23 (ref 5)	5.2	7.8
298	5.7 (ref 1), 5.90 (ref 2), 5.19 (ref 3), 5.65 (ref 5)	5.6 ± 0.3 (R)	8.4 (R)
308	6.21 (ref 5)	6.2	9.3
318	6.93 (ref 5)	6.9	10

α Obtained by averaging where appropriate; σ_n has no statistical
 <u>significance</u>. (continued next page)

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COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C<sub>9</sub>H<sub>12</sub>;

[95-63-6]

(2) Water; H<sub>2</sub>O; [7732-18-5]

August 1985
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CRITICAL EVALUATION: (continued)

REFERENCES

- 1. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75.
- 2. Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u>, 20, 320-2.
- 3. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 4. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 5. Sanemasa, I.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

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COMPONENTS:

McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267-75.
PREPARED BY:
A. Maczynski, Z. Maczynska, and A. Szafranski
zene in water at 25°C was reported tole fraction, x_1 , calculated g sln and 8.5 x 10 ⁻⁶ .
INFORMATION
SOURCE AND PURITY OF MATERIALS:
<pre>(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 4 g(1)/10⁶ g(2) (standard deviation of mean) REFERENCES:</pre>

ORIGINAL MEASUREMENTS:

172	38_128
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene; C ₉ H ₁₂ ;	Sutton, C.; Calder, J.A.
[95-63-6]	J. Chem. Eng. Data 1975, 20, 320-2.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of 1,2,4-trimethylben:	zene in water at 25°C was reported
to be 59.0 mg(1)/kg(2). The correspo	onding mass percent and mole fraction,
x_1 , calculated by the compilers are (.00590 g(l)/100 g sln and
8.83×10^{-6} .	
}	

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.8 mg(1)/kg(2) (the standard deviation of the
	mean for six replicates)
	REFERENCES:
	l

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,4-Trimethylbenzene; C₉H₁₂; [95-63-6] (2) Water; H₂O; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C and at system pressure was reported to be 51.9 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00519 g(1)/100 g sln and 7.77 x 10⁻⁶.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<pre>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 1.2 mg(1)/kg(2) REFERENCES:</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,4-Trimethylbenzene; C₉H₁₂;</pre>	Krzyzanowska, T.; Szeliga, J.
[95-63-6]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
(,	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,2,4-trimethylbenz	vene in water at 25°C was reported
to be 51.9 mg(1)/kg(2).	sene in water at 25 C was reported
	ale fraction a calculated
The corresponding mass percent and mo	
by compiler are 0.00519 g(1)/100 g sl	In and 7.78×10^{-1} .
Editor's Note: Based on the results	for this and other hydrocarbon-water
systems, uncertainity exists about wh	_
independent of that of Price for the	same system (see previous page).
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in	(1) not specified.
(2) were prepared in two ways. First, 200 µL of (1) was injected	(2) not specified.
into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)	
and (2) as above was thermostatted at 70°C and then cooled to 25°C. The	a
time required to obtain equilibrium was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-ll gas chromat-	
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat- urated solutions of heptane in (2)	soly. 1.6 mg(1)/kg(2) (standard
were used as standard solutions.	deviation from 7-9 determinations).
	REFERENCES:

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COMPONENTS:		ORIGINAL MEASUREMENTS:	
[95-63-6]	thylbenzene; C ₉ H ₁₂ ;	Sanemasa, I.; Araki, Deguchi, T.; Nagai, Bull. Chem. Soc. Jpn. <u>1</u>	н.
(2) Water; H ₂ O;	[7732-18-5]	Date. crem. Doc. opr.	<u></u> ,, 1034-02.
VARIABLES:		PREPARED BY:	
Temperature: 15	-45°C	G.T. Hefter	
EXPERIMENTAL VALUES	3: e solubility of 1,2,4-t	rimethylbenzene in wa	ter
t /°C	10 ⁴ mol(1)/dm ³ sln	10 ³ g(1)/100 g sln (compiler) ^a	10 ⁶ x ₁ (compiler) ^a
15	4.35 ± 0.12	5.23	7.84
25	4.69 ± 0.07	5.65	8.48
35	5.14 ± 0.20	6.21	9.32
45	5.71 ± 0.07	6.93	10.4
a			
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/P	ROCEDURE:	SOURCE AND PURITY OF MAT	ERIALS:
100-200 cm ³ of (liquid (1) were but connected th	s similar to an ref 2) and is ail in the paper. 2) and 10-20 cm ³ of placed in separate ermostatted flasks. uilibrium was estab-	purity 95.0%, u further purific	nd. Ltd.), stated sed without
was a recircu to transport vapo	llating strea Prapo ^{li} to the flask Five 10 cm ³ aliquots		
funnels. The co (2) was then det into chloroform spectrophotometr spectrophotometr	ncentration of (1) in ermined by extraction followed by UV- Ty. Standards for the Ty were prepared by	ESTIMATED ERROR: soly. see table, typ specified. temp. ± 0.01°C.	e of error not
weight from pure	liquid solutes.	REFERENCES :	
		1. Kell, G.S. J. Chem. Eng. Data	
		2. Sanemasa, I.; Ar Deguchi, Y.; Nag Chem. Lett. <u>1981</u> ,	ai, H.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene;	Sutton, C.; Calder, J.A.
C ₉ H ₁₂ ; [95-63-6]	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
(2) Artificial seawater (ref l)	
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of 1,2,4-trimethylben	zene in artificial seawater is
reported to be 39.6 mg(l)/kg sln. T	he corresponding mass percent and
mole fraction, x_1 calculated by the	compiler are 3.96 x 10 ⁻³ g(1)/100 g
_	ificial seawater composition of ref 1.
	Í
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was	(1) from either Aldrich Chemical
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and
through the vapor phase. The	Bell, 99+% pure.
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	-
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.5 (std. dev.)
	REFERENCES: 1. Lyman, J.; Fleming, R.H.; J. Mar. Res. 1940, 3, 135.

38_133

COMPONENTS:	EVALUATOR:
<pre>(1) Mesitylene; C₉H₁₂; [108-67-8] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	August 1985

CRITICAL EVALUATION:

Quantitative solubility data for the mesitylene (1) - water (2) system have reported in the publications listed in Table 1.

	and the second	olubility Studie ater (2) System	es of
REFERENCE	Т/К	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	residue volume
Andrews and Keefer (ref 2)	298	(l) in (2)	spectrophotometric
Guseva and Parnov (ref 3)	391-484	(l) in (2)	unspecified
Englin et al. (ref 4)	293-313	(2) in (1)	analytical
Sutton and Calder (ref 5)	298	(1) in (2)	GLC
Sanemasa $et \ al$. (ref 6)	288-318	(1) in (2)	spectrophotometric
Sanemasa <i>et al</i> . (ref 7)	288-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF MESITYLENE (1) IN WATER (2)

All the available data on the solubility of mesitylene in water at low temperatures (288-318K) are summarized in Table 2, except for the rejected values referred to below.

At 298K, the only temperature where comparison is possible, the datum of Sutton and Calder (ref 5) is in good agreement with the values reported by Sanemasa *et al.* (ref 6,7) enabling the mean to be Recommended. The datum of Andrews and Keefer (ref 2) is markedly higher than the other studies (ref 5,6,7) and is rejected as is the approximate value of Booth and Everson (ref 1).

At other temperatures only the two data sets of Sanemasa $et \ al$. (ref 6,7) are available and must thus be considered as Tentative.

At the elevated temperatures (*ca.* 390-480K) and system pressure only the data of Guseva and Parnov (ref 3) are available and thus no Critical Evaluation is possible. However, it may be noted that solubilities reported by Guseva and Parnov are not always reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

(continued next page)

COMPONENTS :	EVALUATOR:
(2) Water: H_O: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	August 1985.

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (R) and Tentative Values of the Solubilityof Mesitylene (1) in Water (2)

T/K	Solubility	values
	Reported values	"Best" values $(\pm \sigma_n)$
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln 10 ⁶ x ₁
288	4.56 (ref 6), 4.60 (ref 7)	4.6 6.9
298	4.82 (ref 5), 4.95 (ref 6) 5.00 (ref 7)	$4.89 \pm 0.08^{a}(R)$ 7.4 (R)
308	5.42 (ref 6), 5.49 (ref 7)	5.4 8.2
318	5.65 (ref 6), 5.89 (ref 7)	5.7 8.7

a Obtained by simple averaging; σ_n has no statistical significance.

2. THE SOLUBILITY OF WATER (2) IN MESITYLENE (1)

The solubility of water in mesitylene has been reported only by Englin $et \ al$. (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for experimental values. However, it may be noted that for other hydrocarbon systems studies by Englin $et \ al$. their results are generally reliable at T < 300K but are higher than Recommended values at higher temperatures.

REFE RENCES

1.	Booth, H.S.; Everson, H.E. Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
2.	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
3.	Guseva, A.N.; Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9.
4.	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
5.	Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
6.	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Chem. Lett. <u>1981</u> , 225-8.
7.	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.
8.	Alwani, Z.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. <u>1969</u> , 73, 294-301.
NOTE	ADDED IN PROOF
Alwan	i and Schneider (ref 8) have also reported a critical locus of the
mesit	ylene-water system.

30_134	175
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Booth, H.S.; Everson, H.E.
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of mesitylene in water was reported to be less than 0.02 g()	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant- temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes and then centrifuged for 5 minutes. After this treatment, the volume of residue was determined	 (1) source not specified; CP or highest commercial grade; used as received. (2) distilled.
directly.	<pre>soly. ± 0.1 mL(1)/100 mL(2). REFERENCES:</pre>

Components :	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
	A. Mozynski und z. Mozynski
EXPERIMENTAL VALUES:	
The solubility of mesitylene in wate to be 0.0097 g(l)/100 g sln.	r at 25°C was reported
The corresponding mole fraction, x_1 , is 1.45 x 10 ⁻⁵ .	calculated by the compilers
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a	<pre>(1) Eastman Kodak Co. white label; fractionally distilled;</pre>
constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous	b.p. 165.0°C.
phase was withdrawn and extracted with a measured volume of hexane	(2) not specified.
(10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next,	
the absorbance of the hexane phase was measured against a hexane	
blank on the Beckman spectrophoto- meter.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

38_136	18
COMPONENTS: (1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	ORIGINAL MEASUREMENTS: Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.
VARIABLES:	PREPARED BY:
Temperature: 118-211°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	•
Solubility of me	esitylene in water
<i>t/°C</i> g(1)/100 g	$\frac{10^4 x_1}{(\text{compiler})}$
118 0.007	0.10 0.19
144 0.013 187 0.041 211 0.078	0.61 1.17
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS: (1) source not specified;
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n_D^{20} 1.49945.
	(2) doubly distilled.
	ESTIMATED ERROR:
	not specified.

REFERENCES:

		ORIGINAL MEASUREMENTS:
(l) Mesitylene; C ₉ H ₁₂ ; (2) Water· H ₂ O; [7732·		Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
		Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42- 6.
VARIABLES:		PREPARED BY:
Temperature: 20-40°C		A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:		
Solut	oility of Wat	er in Mestitylene
<u>t/°C</u>	g(2)/100 g sl	$\frac{10^3 x_2}{(\text{compiler})}$
20 30	0.0291 0.0393	1.94 2.62
40	0.0519	3.45
- 		_
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
Component (1) was introd	luced into a	
Component (1) was introc thermostatted flask and for 5 hr. with (2). Nex	luced into a saturated <t, calcium<="" td=""><td>SOURCE AND PURITY OF MATERIALS:</td></t,>	SOURCE AND PURITY OF MATERIALS:
Component (1) was introd thermostatted flask and for 5 hr. with (2). New hydride was added and th hydrogen volume measured	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR:
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Ney hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.
Component (1) was introd thermostatted flask and for 5 hr. with (2). Nex hydride was added and th hydrogen volume measured the concentration of (2)	duced into a saturated kt, calcium he evolving d and hence	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C ₉ H ₁₂ ; [108-67-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of mesitylene in water	r at 25°C was reported to be
48.2 mg(l)/kg(2). The corresponding	mass percent and mole fraction,
x_1 , calculated by the compilers are (0.00482 g(l)/l00 g sln and
7.22×10^{-6} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(2) Water: H_O; [7732-18-5]		Sanemasa, I.; Araki, M.; Deguchi Nagai, H. <i>Chem. Lett.</i> <u>1981</u> , 225-8.	, T.;
VARIABLES:		PREPARED BY:	
Temperature: 15-45°C		M.C. Haulait-Pirson	
EXPERIMENTAL VALUE	:S:		
	Solubility of mesi	tylene in water	
t/°C	g(1)/L	$\frac{g(1)}{100 \text{ g sln}^{a}} = \frac{10^{6} x_{1}^{a}}{10^{6} x_{1}^{a}}$	
15	0.0456 ± 0.0010	0.00456 6.82	
25	0.0495 ± 0.0015	0.00495 7.41	
35	0.0542 ± 0.0033	0.00542 8.11	
45	0.0565 ± 0.0031	0.00565 8.46	
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/	PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, gen- erated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/ min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reser- voir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at con-		<pre>(1) analytical reagent grade use purchased. (2) redistilled. ESTIMATED ERROR: soly. : given above REFERENCES:</pre>	d as
stant solvent temperature. Solubil- ity values were calculated from Henry's law constants.			

COMPONENTS :		
	ORIGINAL MEASUREMENTS:	
(1) Magitulana (1.2 Ermminathula	Sanemasa, I.; Araki,	М.;
(1) Mesitylene (1,3,5-Trimethyl-	Deguchi, T.; Nagai, I	
benzene); C ₉ H ₁₂ ; [108-67-8] (2) Water; H ₂ O; [7732-18-5]	Bull. Chem. Soc. Jpn. 1	
(2) water, "20," [7,52 10 5]		
VARIABLES:	PREPARED BY:	
Temperature: 15-45°C	G.T. Hefter	
EXPERIMENTAL VALUES:		
The solubility of 1,3,5-	trimethylbenzene in wat	er
$t/^{\circ}$ C 10 ⁴ mol(1)/dm ³ sln	10^3 g(1)/100 g sln	$10^{6} x_{1}$
	(compiler) ^a	(compiler) ^a
15 3.83 ± 0.15	4.60	6.90
25 4.15 ± 0.22	5.00	7.50
35 4.55 ± 0.23	5.49	8.22
45 4.85 ± 0.32	5.89	8.83
AUXILIARY	INFORMATION	
	INFORMATION SOURCE AND PURITY OF MATER	IALS :
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an	SOURCE AND PURITY OF MATER	ent grade (Wako
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In	ent grade (Wako d. Ltd.), stated
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of	SOURCE AND PURITY OF MATER	ent grade (Wako d. Ltd.), stated ed without
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks.	 SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no 	ent grade (Wako d. Ltd.), stated and without tion.
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab-	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica	ent grade (Wako d. Ltd.), stated sed without tion.
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and	 SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no 	ent grade (Wako d. Ltd.), stated sed without tion.
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask	 SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. 	ent grade (Wako d. Ltd.), stated sed without tion.
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory	SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given.	ent grade (Wako d. Ltd.), stated ed without tion.
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots	 SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. 	ent grade (Wako d. Ltd.), stated ed without tion. further details
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, type specified.</pre>	ent grade (Wako d. Ltd.), stated ed without tion. further details
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, type specified: temp. ± 0.1°C.</pre>	ent grade (Wako d. Ltd.), stated ed without tion. further details
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, type specified. temp. ± 0.1°C. REFERENCES:</pre>	ent grade (Wako d. Ltd.), stated ed without tion. further details
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was estab- lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by	<pre>SOURCE AND PURITY OF MATER (1) Analytical reage Pure Chemical In purity 97.0%, us further purifica (2) Redistilled; no given. ESTIMATED ERROR: soly. see table, type specified: temp. ± 0.1°C.</pre>	ent grade (Wako d. Ltd.), stated eed without tion. further details

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Mesitylene (1,3,5-Trimethyl- benzene); C₉H₁₂; [108-67-8] (2) Artificial seawater (ref 1) 	Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	

The solubility of 1,3,5-trimethylbenzene in artificial seawater is reported to be 31.3 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 3.13 x 10^{-3} g(1)/100 g sln and 4.81 x 10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.	 from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. made from doubly distilled water and salts 99+% pure.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.2 (std. dev.)
	REFERENCES:
	<pre>1. Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.</pre>

COMPONENTS:	EVALUATOR:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

CRITICAL EVALUATION:

Quantitative solubility studies of the cumene (1) - water (2) system have been reported in the publications listed in Table 1.

	(2)		
Reference	T/K	Solubility	Method
Stearns et al. (ref 1)	298	(1) in (2)	turbidimetric
Andrews and Keefer (ref 2)	298	(l) in (2)	spectrophotometric
Glew and Robertson (ref 3)	298-354	(l) in (2)	spectrophotometric
McAuliffe (ref 4)	298	(1) in (2)	GLC
Englin <i>et al</i> . (ref 5)	273-323	(2) in (1)	analytical
McAuliffe (ref 6)	298	(l) in (2)	GLC
Sutton and Calder (ref 7)	298	(l) in (2)	GLC
Price (ref 8)	298	(l) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa <i>et al</i> . (ref 10)	288-318	(l) in (2)	spectrophotometric

TABLE 1: Quantitative Solubility Studies ofthe Cumene (1) - Water (2) System

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF CUMENE (1) IN WATER (2)

With the exception of the rejected values referred to below and the datum of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) all the available data on the solubility of cumene in water are summarized in Table 2.

At 298K where the most data are available, agreement is only fair. The values of Stearns *et al.* (ref 1), Andrews and Keefer (ref 2) and Glew and Robertson (ref 3) are much higher than other studies (ref 4,6,7,8,10) and are rejected.

At other temperatures the values of Glew and Robertson are again in only fair agreement with those of Sanemasa $et \ al$. (ref 10), but in the absence of confirmatory studies it is not possible to express a preference for either data set, and the averaged "Best" values should be regarded as Tentative. Selected data are also plotted in Figure 1

(continued next page)

EVALUATOR: **COMPONENTS:** (1) Cumene; C₉H₁₂; [98-82-8] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. January 1986. CRITICAL EVALUATION: (continued) Tentative Values of the Solubility of TABLE 2: Cumene (1) in Water (2) T/K Solubility values Reported values^a "Best" values $(\pm \sigma_n)^b$ $10^{3} g(1) / 100 g sln$ 10³g(1)/100g sln $10^5 x_1$ 5.95 (ref 10) 288 0.90 6.0 298 5.3 (ref 4), 5.0 (ref 6), 5.6 ± 0.7 0.84 6.53 (ref 7), 4.83 (ref 8), 6.15 (ref 10) 7.4 ± 0.9 303 8.3* (ref 3), 6.5* (ref 10) 1.11 8.2 ± 0.9 1.23 313 9.0* (ref 3), 7.3* (ref 10) 323 10.0* (ref 3), 8.0* (ref 10) 9 ± 1 1.3 12 333 11.5* (ref 3) 1.8 343 13.5* (ref 3) 14 2.1 16.1* (ref 3) 353 16 2.4 a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data. b Obtained by averaging where appropriate; σ_n has no statistical significance. 360 350 340 £ 330 Temperature 320 310 300 290

COMPONENTS :	EVALUATOR:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

CRITICAL EVALUATION: (continued)

Interestingly, application of the van't Hoff equation to both data sets gives values of $\Delta H_{sln} = 3.5$ (ref 3) and 5.1 (ref 10) kJ mol⁻¹ and $\Delta C_{p,sln} = 291$ (ref 3) and 382 (ref 10) J K⁻¹ mol⁻¹. Comparison of these values with those of related systems suggests both solubility data sets are reasonable.

2. THE SOLUBILITY OF WATER (2) IN CUMENE (1)

Quantitative solubilities of water in cumene have been reported only in the study of Englin *et al*. (ref 5) and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet following this Critical Evaluation for the experimental values. However, it may be noted that for other hydrocarbon systems studied by these authors, the data of Englin *et al*. are generally reliable at T < 300K but higher than Recommended values at higher temperatures.

REFERENCES

- Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkin, L.D. J. Chem. Phys. <u>1947</u>, 15, 496-507.
- 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u>, 72, 5034-7.
- 3. Glew, D.N.; Robertson, R.E. J. Phys. Chem. 1956, 60, 332-7.
- 4. McAuliffe, C. Nature 1963, 200, 1092-3.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1966</u>, 10, 1267-75.
- 6. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75.
- 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data <u>1975</u>, 20, 320-2.
- 8. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 9. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 10. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for graphics and regression analyses.

38_143
ORIGINAL MEASUREMENTS:
Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D.
J. Chem. Phys. <u>1947</u> , 15, 496-507.
PREPARED BY:
A. Maczynski and D. Shaw
25°C was reported to be calculated by the compiler
INFORMATION
SOURCE AND PURITY OF MATERIALS:
(1) not specified.(2) not specified.
ESTIMATED ERROR:
temp. ± 3°C.
REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ 0; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of cumene in water at to be 0.0073 g(l)/l00 g sln.	25°C was reported
The corresponding mole fraction, x_1 ,	calculated by the compilers
is 1.09×10^{-5} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous Phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.	 (1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 151.5-152.0°C. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :			ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]		31	Glew, D.N.; Robertson, R.E.
, 			J. Phys. Chem. 1956, 60, 332-7.
(2) Water; H ₂ O; [7732-18-5]			5. rnys. chem. <u>1956</u> , 60, 552-7.
VARIABLES:			PREPARED BY:
Temperature:	298-353 К		A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES	S:		
	Solu	bility of	cumene in water
		5	g(l)/100 g sln
	т/к	$\frac{10^5 x_1}{x_1}$	(compiler)
	298.086	1.2050	0.00804
	303.134 308.068	1.2416 1.2825	0.00829 0.00856
	313.108 318.055	1.3446 1.4162	0.00897 0.00945
	323.052	1.5037	0.01004
	328.066 333.133	1.6011 1.7221	0.01069 0.01149
	338.315 343.470	1.8624 2.0302	0.01243 0.01355
	348.247	2.2064	0.01472
	353.359	2.4212	0.01616
		AUXILIARY	INFORMATION
METHOD/APPARATUS/P	ROCEDURE:		SOURCE AND PURITY OF MATERIALS:
Component (1) was floated on the surface of the main body of the water and the aqueous solution was pumped steadily in a closed circuit through the quartz absorption cell where its absorbance was measured. From these values the solubility of (1) in (2) was calculated.		the ion was circuit on cell asured. ility	 (1) Eastman Kodak Co. White Label; distilled in an atmosphere of nitrogen; b.p.range 0.2°C, passed repeatedly through a fresh column of Fisher activated alumina, (2) distilled; passed through a demineralizing column. ESTIMATED ERROR: temp. ± 0.002 K soly. ± 1.00% at 25°C and ± 1.25% at 80°C (standard error) REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) 1963, 200, 1092-3.
(2) water, "20, [//32-10-5]	<i>Nature</i> (<i>Donabh</i>) <u>1903</u> , 200, 1092-5.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
-	
EXPERIMENTAL VALUES:	
The solubility of cumene in water at	25°C was reported
to be 0.0053 g(1)/100 g sln.	
The corresponding mole fraction, x_1 ,	calculated by the compilers
is 7.9 x 10 ⁻⁶ .	
-	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in	(1) Phillips Petroleum Co.; 99+%; used as received.
(2) was prepared by either shaking vigorously on a reciprocal shaker	
or stirring for several days with a magnetic stirrer.	(2) distilled.
A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was	
injected directly into a gas liquid chromatograph.	
	ESTIMATED ERROR:
	temp. ± 1.5°C
	soly. 0.0005 (standard deviation of mean)
	REFERENCES:
	1 1

154	50_147
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of W	Nater in Cumene
$t/^{\circ}C$ g(2)/100 g sln	<u>10³ <i>x</i>2</u> (compiler)
0 0.0156	1.04
10 0.0219	1.46 2.02
20 0.0303 30 0.0407	2.02
40 0.0550 50 0.0710	3.66 4.72
	7.72
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving	(27 Not Specifica.
hydrogen volume measured and hence the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	ALF LAENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1966</u> , 70, 1267-75.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of cumene in water at to be 50 g(1)/10 ⁶ g(2). The corresponding mass percent and m by the compilers are 0.0050 g(1)/100	nole fraction, x_1 , calculated

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	 Phillips Petroleum or Columbia Chemical; used as received. distilled. 	
	ESTIMATED ERROR:	
	<pre>temp. ± 1.5°C soly. 5 g(1)/10⁶ g(2) (standard deviation of mean)</pre>	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of cumene in water at	25°C was reported to be
65.3 mg(1)/kg(2). The corresponding	
x_1 , calculated by the compilers are	-
9.78 x 10^{-6} .	
9.78 x 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.8 (the standard deviation of the mean for six replicates)
	REFERENCES :

ORIGINAL MEASUREMENTS:
Price, L.C.
Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
PREPARED BY:
M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C and at system pressure was reported to be 48.3 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00483 g(l)/l00 g sln and 7.23 x 10⁻⁶.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many de- tails are given in the paper.	<pre>(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. ± 1°C soly. ± 1.2 mg(1)/kg(2) REFERENCES:</pre>	

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Krzyzanowska, T.; Szeliga, J.	
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of cumene in water at 25°C was reported		
to be 48.3 mg(1)/kg(2).		
The corresponding mass percent and mole fraction, x_1 , calculated		
by compiler are 0.00483 g(1)/100 g sln and 7.24 x 10^{-6} .		

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	(1) not specified.(2) not specified.	
	ESTIMATED ERROR: soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).	
	REFERENCES:	

ORIGINAL MEASUREMENTS:
Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.
PREPARED BY:
G.T. Hefter
ropylbenzene in water
$\begin{array}{ccc} 10^{3} \text{ g(1)/100 g sln} & 10^{6} x_{1} \\ \text{(compiler)}^{a} & \text{(compiler)}^{a} \end{array}$
5.95 8.92
6.15 9.22
6.87 10.3
7.75 11.6
INFORMATION
SOURCE AND PURITY OF MATERIALS:
 Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification. Padiatillade as further details
(2) Redistilled; no further details given.
ESTIMATED ERROR:
soly. see table, type of error not specified. temp. ± 0.01°C.
REFERENCES:
 Kell, G.S. J. Chem. Eng. Data <u>1975</u>, 20, 97.
 Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. <u>1981</u>, 225-8.

200	38_153	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Cumene; C ₉ H ₁₂ ; [98-82-8]	Sutton, C.; Calder, J.A.	
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.	
VARIABLES: One temperature: 25.0°C	PREPARED BY:	
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt	
EXPERIMENTAL VALUES:		
The solubility of cumene (isopropylb	enzene) in artificiąl seawater is	
reported to be 42.5 mg(1)/kg sln. T	he corresponding mass percent and	
mole fraction, x_1 calculated by the	compiler are 4.25 x 10 ⁻³ g(1)/100 g	
sln and 6.54 x 10^{-6} assuming the artificial seawater composition of		
ref 1.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration	(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.	
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled	
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.	
entomatography.		
	ESTIMATED ERROR:	
	temp. ± 0.1°C	
	soly. 0.2 (std. dev.)	
	REFERENCES: 1. Lyman, J.; Fleming, R.H.;	
	J. Mar. Res. <u>1940</u> , 3, 135.	

COMPONENTS:	EVALUATOR:
<pre>(1) Propylbenzene, C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Sanemasa et al. (ref 9)

Quantitative solubility data for propylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in propylbenzene.

TABLE 1: Quantitative Solubility Studies ofPropylbenzene (1) in Water (2)		
Reference	T/K	Method
Fühner (ref 1)	288	volumetric
Stearns et al. (ref 2)	298	turbidimetric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Guseva and Parnov (ref 5)	359-495	synthetic
Krasnoshchekova and Gubergrits (ref 7)	298	GLC
Sanemasa <i>et al</i> . (ref 8)	288-318	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

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Guseva and Parnov (ref 5) have reported solubility data for propylbenzene in water at elevated temperatures (359-495K) and system pressure. Alwani and Schneider (ref 6) have studied phase equilibria in the propylbenzene water system at 600-678K and 20-200 MPa. In the absence of confirmatory studies no Critical Evaluation of these data is possible; however, it may be noted that data reported by Guseva and Parnov (ref 5) for other hydrocarbon - water systems are generally not reliable. The interested user is referred to the relevant Data Sheets for experimental results.

All other data for the solubility of propylbenzene in water are summarized in Table 2 except for the 298K data of Fühner (ref 1) and Klevens (ref 4) which are very much higher than all other studies (ref 3,7,8,9) and are The remaining data at 298K, the only temperature where comparirejected. son is possible, are in only fair agreement.

At other temperatures only the values of Sanemasa $et \ al.$ (ref 8) are available. Thus all solubility values in Table 2 must be considered Tentative.

(continued next page)

spectrophotometric

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COMPO	NENTS:	EVALUATOR:	
(1)	Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	G.T. Hefter, School of Mathematical	
	<i>,</i> 12	and Physical Sciences, Murdoch	
(2)	Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia.	
		March 1986.	
CRITI	CAL EVALUATION: (continued)		
	<u>TABLE 2: Tentative Va</u> Propylbenzene (<u>lues of the Solubility of</u> 1) in Water (2)	
Т/К	T/K Solubility values		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln 10 ⁶ x ₁	
288	4.66 (ref 8)	4.7 7.0	
298	5.5 (ref 3), 7.0 (ref 7)	5.5 ± 0.9 8.2	
308	5.10 (ref 8), 4.52 (ref 9) 5.50 (ref 8)	5.5 8.2	
318	6.41 (ref 8)	6.4 9.6	
	otained by averaging where appropr	iate; σ_n has no statistical signifi-	
REFE	ERENCES		
1.	Fuhner, H. Chem. Ber. 1924, 57	, 510-4.	
2. Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, L.D. J. Chem. Phys. 1947, 15, 496-507.			
з.			
4.			
5.			
6.			
7.			
8.			
9.	9. Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc.		
	Jpn. <u>1984</u> , 57, 1539-44.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Propylbenzene; C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5]</pre>	Fuhner, H. Ber. Dtsch. Chem. Ges. 1924, 57, 510-5.
VARIABLES:	PREPARED BY:
One temperature: 15°C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa 0.006 g(l)/100 g sln. The corresponding mole fraction, x_1 , is 9 x 10 ⁻⁶ .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm ³ (2) until a	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; commercial grade; used as received,</pre>
completely clear solution was no longer obtained at the experimental temperature.	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

204	38_156
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Phys. <u>1947</u> , 15, 496-507.
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa 0.012 g(1)/100 g sln. The corresponding mole fraction, x_1 , is 1.8 x 10 ⁻⁵ .	

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility. (1) not specified. ESTIMATED ERROR: ESTIMATED ERROR: temp. ± 3°C. REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Andrews, L.J.; Keefer, R.M.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034 - 7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of propylbenzene in water at 25°C was reported to be 0.0055 g(l)/100 g sln.		
The corresponding mole fraction, x_1 , is 8.2 x 10 ⁻⁶ .	calculated by the compilers	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas- ured against a hexane blank on the Beckman spectrophotometer.	 (1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 157.8-158.1°C. (2) not specified. 	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

206	38_158	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Klevens, H.B.	
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.	
VARIABLES:	PREPARED BY:	
Temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of propylbenzene in wa 0.12 g(1) L ⁻¹ sln and 0.001 mol(1)		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility of (1) in (2) was determined by shaking small amounts	(1) not specified.	
of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(2) not specified.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES :	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. <u>1964</u> , 38, 805-6.
VARIABLES: Temperature: 85.8-222.0°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: Solubility of propylbenzene in water	
<i>t/°C</i> g(1)/100 g	$sln = \frac{10^5 x_1}{2}$ (compiler)

	g(1)/100 g SIN	$\frac{10 x_1}{1}$ (complicity)
85.8	0.0132	1.98
114.5	0.0166	2.49
140.5	0.0321	4.81
188.0	0.087	13.04
222.0	0.245	36.8

AUXILIARY INFORMATION	
ETHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The measurements were made in	(1) not specified.
sealed glass tubes. No details were reported in the paper.	(2) not specified.
	ESTIMATED ERROR:
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

-	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C ₉ H ₁₂ ; [103-65-1]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Water; H ₂ O; [7732-18-5]	Vodnye. Resursy. <u>1975</u> , 2, 170-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of propylbenzene in wa to be 0.070 mg(1) cm ⁻³ sln. The corresponding mass percent and mo by the compiler are 0.0070 g(1)/100 g assumption that 1.00 cm ⁻³ sln = 1.00	ble fraction, x_1 , calculated g sln and 1.05 x 10 ⁻⁵ . The
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	(1) described in ref (1).
The solubility of (1) in (2) was determined by glc.	
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 1°C
	REFERENCES :
	<pre>1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya 1973, 13, 885.</pre>

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Propylbenzene; C₉H₁₂; [103-65-1] Sanemasa, I.; Araki, M.; (2) Water; H₂O; [7732-18-5] Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62. VARIABLES: PREPARED BY: Temperature: 15-45°C G.T. Hefter EXPERIMENTAL VALUES: The solubility of propylbenzene in water 10⁶ *x* 1 10^3 g(1)/100 g sln $10^4 \text{ mol}(1)/\text{dm}^3 \text{ sln}$ t /°C (compiler)^{*a*} (compiler)^a 6.99 4.66 3.88 ± 0.15 15 7.64 25 4.23 ± 0.12 5.10 35 4.55 ± 0.07 5.50 8.25 9.61 45 5.28 ± 0.17 6.41 а Assuming solution densities to be the same as those of pure water at the same temperature (ref 1). AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), no (1) The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. $100-200 \text{ cm}^3$ of (2) and $10-20 \text{ cm}^3$ of stated purity, used without further purification. liquid (1) were placed in separate Redistilled; no further details but connected thermostatted flasks. (2) After thermal equilibrium was estabgiven. lished a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 a were withdrawn into separatory Five 10 cm³ aliquots ESTIMATED ERROR: The concentration of (1) in funnels. (2) was then determined by extraction soly. see table, type of error not into chloroform followed by UVspecified. spectrophotometry. Standards for the temp. ± 0.1°C. spectrophotometry were prepared by weight from pure liquid solutes. **REFERENCES:** 1. Kell, G.S. J. Chem. Eng. Data <u>1975</u>, 20, 97.

 Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. Chem. Lett. <u>1981</u>, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Propylbenzene; C₉H₁₂; [103-65-1] (2) Water; H₂O; [7732-18-5]</pre>	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc. Jpn. <u>1984</u> , 57, 1539-44.
VARIABLES:	PREPARED BY:
One Temperature: 25°C	G.T. Hefter
EXPERIMENTAL VALUES:	

The solubility of propylbenzene in water at 25°C was reported to be $3.76 \times 10^{-4} \mod (1)/\text{dm}^3 \text{ sln.}$ Assuming a solution density of 1.00 kg/dm³ this corresponds to a solubility of $4.52 \times 10^{-3} \text{ g(1)}/100 \text{ g sln}$, $x_1 = 6.78 \times 10^{-6}$, calculated by the compiler.

AUXILIARY INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculat- ing pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectro- photometry.	(1) Analytical reagent grade source and purity not stated, used without further purification.	
	(2) Deionized and redistilled; no further details given.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u> , 55, 1054-62.	

38_163	2
COMPONENTS: (1) 1,8-Nonadiyne; C ₉ H ₁₂ ; [2396-65-8] (2) Water; H ₂ O; [7732-18-5] VARIABLES: One temperature: 25°C EXPERIMENTAL VALUES: The solubility of 1,8-nonadiyne in wa to be 125 g(1)/10 ⁶ g(2). The corresponding mass percent and ma by the compilers are 0.0125 g(1)/100	ble fraction, x_1 , calculated
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	SOURCE AND FURITI OF MATERIALS:

temp.	± 1.5°C
solv.	3 g(1)/10 ⁶ g(2)
-	(standard deviation of mean)

REFERENCES:

212	38_164
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Nonyne; C ₉ H ₁₆ ; [3452-09-3]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. 1966, 70, 1267-75.
(2) water, "20, [//02 10 0]	<u></u> ,,
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski
EXPERIMENTAL VALUES:	
The solubility of 1-nonyne in water at 25°C was reported to be 7.2 g(1)/10 ⁶ g(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00072 g(1)/100 g sln and 1.0 x 10 ⁻⁶ .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromato- graphed in conjunction with a flame- ionization detector.	 (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C soly. 0.5 g(1)/10⁶ g(2)
	(standard deviation of mean) REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Butylcyclopentane; C9H18; [2040-95-1]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water i	n Butylcyclopentane
<u>t/°C</u> <u>g(2)/100 g sln</u>	$10^4 x_2$ (compiler)
10 0.0056 20 0.0095 30 0.0151	3.93 6.66 10.58
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hrs. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.
evaluateu.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,1,3-Trimethylcyclohexane; C9^H18; [3073-66-3] (2) Water; H20; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclohexane in water at 25°C and at system pressure was reported to be 1.77 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.77 x 10^{-4} g(l)/100 g sln and 2.53 x 10^{-7} .

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	 Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. distilled. 		
	ESTIMATED ERROR:		
	temp. ± 1°C		
	soly. ± 0.05 mg(l)/kg(2)		
	REFERENCES:		
	l		

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20_T01	210	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
 1,1,3-Trimethylcyclohexane; 	Krzyzanowska, T.; Szeliga, J.	
С ₉ Н ₁₈ ; [3073-66-3]	Nafta (Katowice), <u>1978</u> , 12, 413 - 7.	
(2) Water; H ₂ O; [7732-18-5]		
-		
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 1,1,3-trimethylcycl to be 0.115 mg(1)/kg(2).	ohexane in water at 25°C was reported	
The corresponding mass percent and mo	ble fraction, <i>m</i> calculated	
by compiler are 1.15×10^{-5} g(1)/100	1	
	,	
Editor's Note: Based on the results systems, uncertainity exists about whether the systems about whether the system of the syste		
independent of that of Price for the	_	
Consequently, this system has not been	en evaluated.	
l		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.	
First, 200 µL of (1) was injected	(2) not specified.	
into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1)		
and (2) as above was thermostatted at 70°C and then cooled to 25°C. The	2	
time required to obtain equilibrium was three weeks. The solubility of		
(1) in (2) was measured by glc. A Perkin-Elmer model F-ll gas chromat-		
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:	
ionization detector was used. Sat- urated solutions of heptane in (2)	soly. 0.02 mg(l)/kg(2) (standard	
were used as standard solutions.	deviation from 7-9 determinations).	
	REFERENCES:	

COMPONENTS:	EVALUATOR:
<pre>(1) 2,2,5-Trimethylhexane; C₉H₂₀; [3522-94-9]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
-	December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,5-trimethylhexane (1) and water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,5-Trimethylhexane (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF 2,2,5-TRIMETHYLHEXANE (1) IN WATER (2)

All the available data on the solubility of 2,2,5-trimethylhexane in water are summarized in Table 2.

At 298K, the only temperature where comparison is possible, the values of McAuliffe (ref 1) and Polak and Lu (ref 2) are in poor agreement (Table 2). The only other value available is that of Polak and Lu at 273K. Thus all solubility values must be regarded as very Tentative in the absence of confirmatory studies.

TABLE 2: Tentative Values of the Solubility of 2,2,5-Trimethylhexane (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁴ g(1)/100g sln	"Best" value 10 ⁴ g(1)/100g sln	s (± σ _n) ^a 10 ⁷ x ₁
273	1.79 (ref 2)	0.8	1.1
298	1.15 (ref 1), 0.54 (ref 2)	0.8 ± 0.3	1.1

a Obtained by averaging where appropriate; σ_{n} has no statistical signigicance.

(continued next page)

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COMPONENTS:	EVALUATOR:
<pre>(1) 2,2,5-Trimethylhexane; C₉H₂₀; [3522-94-9] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2,2,5-TRIMETHYLHEXANE (1)

Only the data of Polak and Lu (ref 2) are available for the solubility of water in 2,2,5-trimethylhexane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values; however, it may be noted that the data of Polak and Lu (ref 2) are generally reliable.

REFERENCES

1. McAuliffe, C. J. Phys. Chem. <u>1966</u>, 70, 1267-75.

2. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23.

the paper.

218	38_169			
Components :	ORIGINAL MEASUREMENTS:			
<pre>(1) 2,2,5-Trimethylhexane; C₉H₂₀; [3522-94-9]</pre>	McAuliffe, C. J. Phys. Chem. <u>1966</u> , 70, 1267 - 75.			
(2) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
One temperature: 25°C	M.C. Haulait-Pirson			
EXPERIMENTAL VALUES:				
The solubility of 2,2,5-trimethylhexane in water at 25°C was reported to be 1.15 mg (1)/kg sln. The corresponding mole fraction, x_1 , calculated by the compiler, is 1.62×10^{-7} . The same value is also reported in ref 1.				
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
In a 250 mL glass bottle, $10-20$ mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) drop- lets. Absence of emulsion was checked microscopically. A 50 µL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the frac- tionator of the gas chromatograph.	 (1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled. ESTIMATED ERROR: temp. ± 1.5°C			
A hydrogen-flame ionization detector was used. Many details are given in	soly. 0.008 mg (1)/kg sln (standard deviation from mean)			

temp. soly.	<pre>± 1.5°C 0.008 mg (1)/kg sln (standard deviation from mean)</pre>
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REFERENCES:

McAuliffe, C. Am. Chem. Soc. Div. Petrol. Chem. <u>1964</u>, 9, 275.

OMPONENTS:		ORIGINAL MEASUREMENT	rs:
[3522-94	imethylhexane; C ₉ H ₂₀ ; -9] ₂ 0; [7732-18-5]	Polak, J.; Lu, Can. J. Chem.	B.C-Y. <u>1973</u> , <i>51</i> , 4018-23.
VARIABLES:		PREPARED BY:	<u></u>
Temperature:	0-25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALU	JES:		
	Solubility of 2,2,5-tri	methylhexane in w	vater
t/°C	mg(1)/kg	g sln	<pre>x1 (compiler)</pre>
	0.79	,c	1.11×10^{-7}
25 ^b	0.79		7.58×10^{-8}
	Solubility of water in	2,2,5-trimethylhe	exane
t/°C	mg(2)/kg	g sln	x ₂ (compiler)
0 ^a	25 ^d		1.78×10^{-4}
25 ^b	75 ^d		5.34 x 10^{-4}
	AUXILIARY	INFORMATION	
determined b The solubili determined b tion. 50 mL 50 mL of (2) mL Hypovial coated rubbe a constant-t The system w ly for 24 hr bath without 7 days befor for analysis	/PROCEDURE: ty of (1) in (2) was y gas chromatography. ty of (2) in (1) was y Karl Fischer titra- of (1) together with were placed in a 125 closed with a Teflon r septum and placed in emperature water bath. as stirred magnetical- or was kept in the stirring for at least e samples were taken . Details of the given in the paper.	grade reage three times water. (2) distilled.	etroleum Co.; pure ent (99%+); shaken s with distilled 2°C; b) ± 0.01°C d) ± 4.7%;
		1	•

220	38_171
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,6-Dimethylheptane; C ₉ H ₂₀ ; [1072-05-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-50°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of Water in	2,6-dimethylbeptane
<u>t/°C g(2)/100 g sl</u>	$\frac{10^4 x_2}{(\text{compiler})}$
10 0.0053	3.77
20 0.0091 30 0.0160	6.48 11.39
40 0.0301 50 0.0465	21.40 33.02
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
	Englin D. A. Disto, A. E. a. Mugolukov	
(1) 2-Methyloctane; C ₉ H ₂₀ ; [3221-61-2]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.	
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.	
VARIABLES:	PREPARED BY:	
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson	
Temperature: 10-30 C	A. Maczynski and M.C. Maurart Firson	
EXPERIMENTAL VALUES:		
Solubility of Water	in 2-methyloctane	
<u>t/°C</u> g(2)/100 g sln	$10^4 x_2$ (compiler)	
10 0.0052 20 0.0090	3.70 6.41	
30 0.0156	11.10	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Component (1) was introduced into a	(1) Not specified.	
thermostatted flask and saturated for 5 hours with (2). Next, calcium	(2) Not specified.	
hydride was added and the evolving	(2) Not Specifica.	
hydrogen volume measured and hence the concentration of (2) in (1) was		
evaluated.		
Į	ESTIMATED ERROR:	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) 3-Methyloctane; C ₉ H ₂₀ ; [2216-33-3]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.			
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.			
VARIABLES:	PREPARED BY:			
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson			
EXPERIMENTAL VALUES:				
Solubility of Water in 3-methyloctane				
<u>t/°C</u> g(2)/100 g s1	$\frac{10^4 x_2}{(\text{compiler})}$			
10 0.0050 20 0.0087 30 0.0155	3.56 6.20 11.03			
AUXILIARY				
	INFORMATION SOURCE AND PURITY OF MATERIALS:			
Component (1) was introduced into a	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Not specified.			
	SOURCE AND PURITY OF MATERIALS:			
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified.			
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified.			
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.			
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR:			

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 4-Methyloctane; C₉H₂₀; [2216-34-4] (2) Water; H₂0; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 4-methyloctane in water at 25°C and at system pressure was reported to be 0.115 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.15 x 10⁻⁵ g(l)/100 g sln and 1.6 x 10⁻⁸.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	 Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. distilled. 		
	ESTIMATED ERROR:		
	temp. \pm 1°C soly. \pm 0.011 mg(1)/kg(2)		
	REFERENCES:		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 4-Methyloctane; C₉H₂₀;</pre>	Krzyzanowska, T.; Szeliga, J.

(2) Water; H₂O; [7732-18-5]

[2216-34-4]

VARIABLES:

One temperature: 25°C M

M.C. Haulait-Pirson

PREPARED BY:

Nafta (Katowice), <u>1978</u>, 12, 413-7.

EXPERIMENTAL VALUES:

The solubility of 4-methyloctane in water at $25^{\circ}C$ was reported to be 0.115 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 1.15 x 10^{-5} g(1)/100 g sln and 1.61 x 10^{-8} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh	(1) not specified.(2) not specified.
Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	soly. 0.02 mg(l)/kg(2) (standard deviation from 7-9 determinations).
urated solutions of heptane in (2)	
urated solutions of heptane in (2)	deviation from 7-9 determinations).
urated solutions of heptane in (2)	deviation from 7-9 determinations).
urated solutions of heptane in (2)	deviation from 7-9 determinations).

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COMPONENTS:	EVALUATOR:
(2) Water: H_{-0} : $[7732-18-5]$	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.
CRITICAL EVALUATION: (continued)	

CRITICAL EVALUATION: (CONTINUED)

TABLE 2. Tentative Solubility Values forNonane (1) in Water (2)

Т/К	Solubility		
	Reported values ^a	"Best" value	$s (\pm \sigma_n)^b$
	10 ⁵ g(1)/100g sln	10 ⁵ g(l)/100g sln	10 ^{8"} "1
293	2.89 (ref 8)	2.9	4.1
298	2.2 (ref 2), 0.71 (ref 5), 1.22 (ref 6), 2.72 (ref 8)	1.7 ± 0.8	2.4
303	1.4* (ref 6)	1.4	2.0
313	l.7* (ref 6)	1.7	2.4
323	2.2* (ref 6)	2.2	3.1
333	2.6* (ref 6)	2.6	3.7
343	3.l* (ref 6)	3.1	4.4
353	3.4* (ref 6)	3.4	4.8
363	3.7* (ref 6)	3.7	5.2
373	4.2* (ref 6)	4.2	5.9
383	8.0* (ref 6)	8.0	11
393	16* (ref 6)	16	22
403	32* (ref 6)	32	45

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the author's original data. b Obtained by averaging where appropriate; σ_n has no statistical signifi-

2. SOLUBILITY OF WATER (2) IN NONANE (1)

Only the single point data of Schatzberg (ref 1) at 298K and Benkovski et al. (ref 3) at 303K are available for the solubility of water in nonane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values; however, it may be noted that the data of Schatzberg (ref 1) are generally reliable.

REFERENCES

cance.

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. McAuliffe, C. Science 1969, 163, 478-9.
- Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. Tr. Inst. Khim. Nefti Prir. Solei Alkad. Nauk Kaz. SSR <u>1970</u>, 2, 25-32.
- 4. Roof, J.G. J. Chem. Eng. Data <u>1970</u>, 15, 301-3.
- 5. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u>, 13, 885-7. (continued next page)

COMPONENTS:	EVALUATOR:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the nonane (1) - water (2) system have been reported in the publications listed in Table 1.

·		*	
Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(l) in (2)	GLC
Benkovski <i>et al</i> . (ref 3)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 5)	298	(1) in (2)	GLC
Price (ref 6)	298-410	(l) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC
Jonsson et al. (ref 8)	288,293	(1) in (2)	partition coeff.

TABLE 1. Quantitative Solubility Studies ofthe Nonane (1) - Water (2) System

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Roof (ref 4) has also reported a three phase critical point of unspecified composition at 555K and 8.5 MPa. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF NONANE (1) IN WATER (2)

All the data available for the solubility of nonane in water are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 7) which does not appear to be independent of that of Price (ref 6) and has therefore been excluded from consideration.

At 298K, the only temperature where comparison is possible, the agreement between the various studies is poor (Table 2) and the average must be regarded as Tentative only. Interestingly, the average value of 1.7×10^{-5} g(1)/100g sln is, however, quite close to the value of 2.0×10^{-5} g(1)g sln predicted by extrapolation of the lower *n*-alkane solubilities.

At other temperatures only the data of Jonsson $et \ al$. (ref 8) at 293K and Price (ref 6) at 303-410K are available and thus no Critical Evaluation is possible. There are also insufficient independent data to warrant plotting.

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COMPONENTS:	EVALUATOR:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

- 6. Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u>, 60, 213-44.
- 7. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- Jonsson, J.A.; Vejrosta, J.; Novak, J. Fluid Phase Equil. <u>1982</u>, 9, 279-86.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
2	
VARIABLES:	PREPARED BY:
One tornersturge 25°C	M.C. Haulait-Pirson
One temperature: 25°C	M.C. Madiait-Filson
EXPERIMENTAL VALUES:	
The solubility of water in nonane at	25°C was reported to be
79 mg(2)/kg sln corresponding to a mo	_
	2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a	(1) Phillips Petroleum Co.; research
layer of (2) in a brown glass bottle	grade; 99.69 mole%; passed
without any agitation. The bottle was sealed with serum cap and com-	repeatedly through a column of silica gel until no absorp-
pletely submerged in the water-bath	tion occurred in the 220 to
for 7 days. A 20-mL sample was withdrawn with a silicone-hydro-	340 nm spectral range.
phobized hypodermic syringe. Sta-	(2) distilled and deionized.
bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was	
used to titrate (2) in (1) directly in the presence of methanol to a	ESTIMATED ERROR:
"dead-stop" end-point using a	temp. ± 0.02°C
Beckman KF3 automatic titrimeter.	soly. 0-6% (deviations from the mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Science 1969, 163, 478-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of nonane in water at	25°C was reported to be
0.220 mg(1)/kg(2).	
The corresponding mass percent and more by the compiler are 2.2 x 10^{-5} g(1)/2	ble fraction, x_1 , calculated
by the complete are 2.2×10^{-3} g(1)/.	100 g Sin and 5.09 x 10 .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with (2). Glass vials were filled with the saturated	(1) not specified.
aqueous phase. Half of water was then displaced and replaced by air.	(2) distilled.
The vials were then sealed and shaker	
for 2 minutes. The gas phase was then displaced through the sample	
loop of a gas chromatograph for analyzing for hydrocarbon content.	
	ESTIMATED ERROR:
	soly. ± 0.021 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR <u>1970</u> , 2, 25-32.
VARIABLES:	PREPARED BY:
One temperature: 303 K	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of water in nonane at 303 K was reported to be 0.0045 g(2)/100 g sln. The corresponding mole fraction, x_2 , value calculated by compiler is 0.00032.	

AUXILIARY	INFORMATION
AUVILIAUI	INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.	(1) source not specified; purified; purity not specified.(2) distilled.
	ESTIMATED ERROR:
	Not specified
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski
EXPERIMENTAL VALUES: The solubility of nonane in water at $x_1 = 1.00 \times 10^{-8}$. The corresponding mass percent calcul 7.1 x 10^{-6} g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10- 12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Price, L.C.
(2) Water; H ₂ O; [7732-18-5]	Ат. Аввос. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
Temperature: 25-136.6°C	F. Kapuku

EXPERIMENTAL VALUES:

.

Solubility of nonane in water at system pressure

t/°C mg(1)/kg(2)		g(l)/100 g sln (compiler)	10 ⁸ x1 (compiler)	
25.0	0.122 ± 0.007	0.0000122	1.71	
69.7	0.309 ± 0.019	0.0000309	4.34	
99.1	0.420 ± 0.034	0.0000420	5.90	
121.3	1.70 ± 0.11	0.000170	23.9	
136.6	5.07 ± 0.25	0.000507	71.2	

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and al- lowed syringe access to the solution	SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; 99+%. (2) distilled. ESTIMATED ERROR: temp. + 1°C			
during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.	solv range of values given above			

COMPONENTS :	ORIGINAL MEASUREMENTS:				
(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Krzyzanowska, T.; Szeliga, J.				
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.				
VARIABLES:	PREPARED BY:				
One temperature: 25°C	M.C. Haulait-Pirson				
EXPERIMENTAL VALUES:					
The solubility of nonane in water at 25°C was reported to be 0.122 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 1.22 x 10 ⁻⁵ g(1)/100 g sln and 1.71 x 10 ⁻⁸ .					

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2)	ESTIMATED ERROR: soly. 0.01 mg(1)/kg(2) (standard
were used as standard solutions.	deviation from 7-9 determinations). REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Nonane; C ₉ H _{2O} ; [111-84-2] (2) Water; H ₂ O; [7732-18-5]	Jonsson, J.A.; Vejrosta, J.; Novak, J. Fluid Phase Equil. <u>1982</u> , 9, 279-86.
VARIABLES:	PREPARED BY:
Temperature: 15-20 ⁰ C	G.T. Hefter
EXPERIMENTAL VALUES:	nonane (1) in water (2)

t/ ^o C	mg(l)/kg sln	l0 ⁵ g(l)/l00g sln (compiler)	10 ⁸ x1 (compiler)	
15	0.289	2.89	4.05	
20	0.272	2.72	3.81	

Solubility values were calculated by the authors from their smoothed air-water partition coefficient ($K_{\rm AW}$) by assuming $K_{\rm AW}$ values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

SOURCE AND PURITY OF MATERIALS:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in ref 1.	 (1) Fluka, > 99%, used as received. (2) Not specified. 			
	ESTIMATED ERROR:			
	Not specified.			
	REFERENCES:			
	 Vejrosta, J.; Novak, J.; Jonsson, J.A. Fluid Phase Equil. <u>1982</u>, 8, 25-35. 			

METHOD/APPARATUS/PROCEDURE:

COMPONENTS:

(1) Nonane; C ₉ H ₂₀ ; [111-84-2]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Seawater	Neftekhimiya <u>1973</u> , 13, 885-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of nonane in seawater	was reported to be
4.3 x 10^{-5} g(1)/100 g sln. and the co	orresponding mole fraction,
$x_1 = 6.0 \times 10^{-8}$.	
AUXILIARY	INFORMATION
LMETHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared	(1) "chemically pure"
by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs.	(2) distilled water plus salt
in a flask placed in a temperature controlled bath. A sample of solu-	mixture.
tion was then transferred to a closed flask with head space volume	
equal to solution volume. Hydro-	
carbon concentration in the head space was determined by gas chroma-	
tography and the corresponding solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

ORIGINAL MEASUREMENTS:

ool of Mathematical ences, Murdoch h, W.A., Australia.

CRITICAL EVALUATION:

Quantitative data for the solubility of naphthalene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Studies of the Solubility of Naphthalene (1) in Water (2)

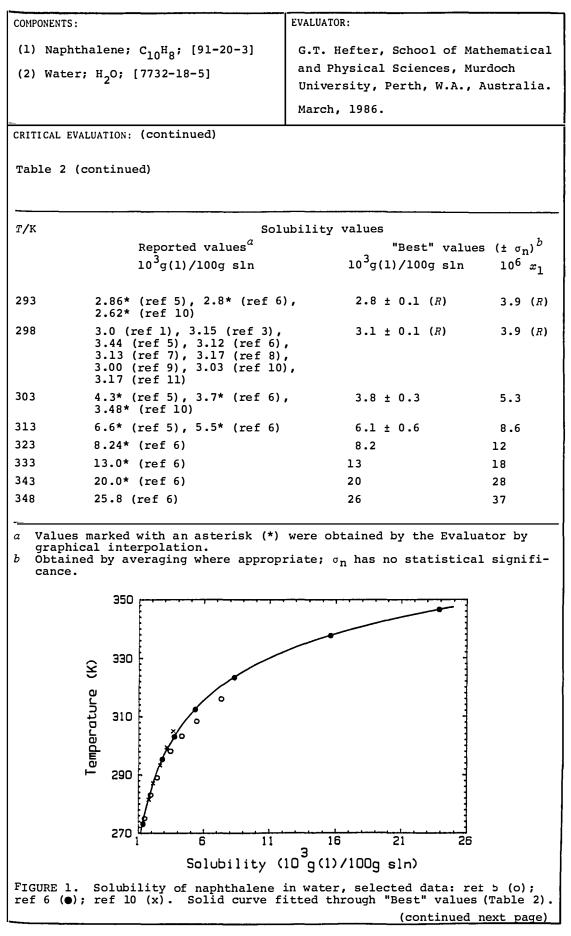
Reference	T/K	Method
Hilpert (ref 1)	273,298	gravimetric
Mitchell (ref 2)	288,298	interferometric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Bohon and Claussen (ref 5)	273-316	spectrophotometric
Wauchope and Getzen (ref 6)	273-348	spectrophotometric
Eganhouse and Calder (ref 7)	298	GLC
Mackay and Shiu (ref 8)	298	spectrofluorometric
Schwarz and Wasik (ref 9)	285-298	spectrophotometric
Schwarz (ref 10)	282-305	spectrophotometric
May et al. (ref ll)	298	HPLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been published on the solubility of water in naphthalene.

Despite the low solubility of naphthalene in water the published data are in excellent agreement. With the exception of the 298K data of Mitchell (ref 2) and Klevens (ref 4) which differ markedly from other studies, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

TABLE 2:	Recommended (of the	Solubility
	of Napht	halene	(1) in Wat	cer (2)		

<i>т/</i> к	Solubility values			
	Reported values ^a "Best" va			
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln	10 ⁶ x1	
273	1.9 (ref 1), 1.37 (ref 5), 1.37 (ref 6)	1.5 ± 0.2	2.1	
283	1.94 (ref 5), 2.0* (ref 6), 1.87* (ref 10)	1.9 ± 0.1 (R)	2.7 (R)	
		(Table 2 continued)	next page)	



EVALUATOR: COMPONENTS: (1) Naphthalene; C₁₀H₈; [91-20-3] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. March, 1986. CRITICAL EVALUATION: (continued) REFERENCES 1. Hilpert, S. Angew. Chem. 1916, 29, 57-9. Mitchell, S. J. Chem. Soc. <u>1926</u>, 129, 1333-6. 2. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-77. з. Klevens, H.B. J. Phys. Chem. 1950, 54, 283. 4. 5. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8. 6. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data 1972, 17, 38-41. 7. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61. 8. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402. 9. Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data 1977, 22, 270-3. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7. 10. 11. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000. ACKNOWLE DGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

38_186	239		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Hilpert, S.		
	Angew. Chem. <u>1916</u> , 29, 57-9.		
(2) Water; H ₂ O; [7732-18-5]	Angew. Chem. <u>1910</u> , 28, 31-9.		
VARIABLES :	PREPARED BY:		
Temperature: 0 and 25°C	A. Maczynski and A. Szafranski		
EXPERIMENTAL VALUES:			
Solubility of naph			
$t/^{\circ}C$ 10 ³	$g(1)/100 g sln = 10^{6} x_{1}$		
0	1.9 2.7		
25	3.0 4.2		
AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A sample of (1) was shaken with	(1) not specified.		
1000 g(2) until saturation and then	_		
filtered. The filtrate was steam distilled to drive away (1) which	(2) not specified.		
was collected and presumably weighed			
	ESTIMATED ERROR:		

not specified.

REFERENCES:

	38_187	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Mitchell, S.	
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. London <u>1926</u> , 1332-6.	
VARIABLES:	PREPARED BY:	
Temperature: 15 and 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of naph	thalene in water	
$\frac{t/^{\circ}C}{d}$ $\frac{g(1) L^{-1}(2)}{d}$ $\frac{g(1)/2}{d}$	100 g sln (compiler) $10^{6}x_{1}$ (compiler)	
15 0.022 0.	0022 3.1	
25 0.040 0.	0040 5.6	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
For this study an interferometer of the type described in ref (1) was constructed.	(1) not specified.(2) not specified.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES :	
	l. Jamin Ann. Chim. Phys. <u>1958</u> , 52, 171.	

COMPONENTS :	
UCALOUFUID:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of naphthalene in wate 0.00315 g(1)/100 g sln. The corresponding mole fraction, x_1 , is 4.42 x 10 ⁻⁶ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea- sured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea- sured against a hexane blank on the	 Eastman Kodak Co., best grade; recrystallized from ethanol; mp. 80.5°C. not specified.
Beckman spectrophotometer.	ESTIMATED ERROR:
	not specified.
	REFERENCES :

242	30_107
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
The solubility of naphthalene in wate 0.0125 g(1) L^{-1} sln and 9.75 x 10^{-5} 1.00 L sln = 1.00 kg sln, the corresp compiler are 0.00125 g(1)/100 g sln a	mol(l) L ⁻¹ sln. Assuming that onding values calculated by the

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Bohon, R.L.; Claussen, W.F.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8.	
VARIABLES:	PREPARED BY:	
Temperature: 0-42.8°C	G.T. Hefter	
EXPERIMENTAL VALUES:		
t/°C 10 ³ g(1),	phthalene in water /100g sln ^a 10 ⁶ x ₁ piler)	
0.0 1. 0.4 1. 0.5 1. 0.9 1. 1.9 1. 9.4 1. 10.0 1. 14.9 2. 15.9 2. 15.9 2. 19.3 2. 25.0 3. 25.6 3. 30.1 4. 30.2 4. 35.2 5. 36.0 5. 42.8 7. ^a Solubilities of (1) in (2) were repor measurements. Solubilities were calc Beer-Lambert law, the stated cell pat "extinction coefficients" (absorptive densities. This gave a solubility of converted to g(1)/l00g sln by assuming ^b Given in the paper as 0.0344g(1)/L si	37 1.92 38 1.94 46 2.05 50 2.11 96 2.75 94 2.72 34 3.29 46 3.45 80, 3.93 44 ^b 4.83 58 5.03 30 6.04 39 6.16 45 7.65 48 7.69 35 10.3 rted as "optical density" (absorbance) culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.	 Allied Chemical & Dye Corp., purified by vacuum distillation. Air-free conductivity water, no other details given. 	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

EXPERIMENTAL VALUES:

mg(l)/kg(2)			•	. 6
t/°C		smoothed with	g(1)/100 g sln	$10^{6}x_{1}$
	experiment	(std dev)	(compiler)	(compile
0.0		13.7(0.2)	0.00137	1.93
22.2	28.8, 29.1, 28.8	28.3	0.00283	3.98
24.5	30.8(2), 30.1(2),	30.7 30.7	0.00307	4.31
25.0		31.2(0.2)	0.00312	4.38
29.9	38.1, 38.2, 38.3	37.3	0.00373	5.24
30.3	38.1, 37.6, 37.6	37.8	0.00378	5.31
	44.6, 43.8	44.3	0.00443	6.23
39.2	52.6, 52.8	53.3	0.00533	7.49
40.1	54.8	55.0	0.00550	7.73
44.7	66.0, 65.5, 65.3	66.2	0.00662	9.30
50.0	•	82.4(0.4)	0.00824	11.58
50.2	78.6	83.1	0.00831	11.68
55.6	106	105	0.0105	14.8
64.5	166, 151, 157	156	0.0156	21.9
73.4	240, 247, 244	239	0.0239	33.6
75.0		258(3)	0.0258	36.3

38_192	245	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Water; H ₂ O; [7732-18-5]	Eganhouse, R.P.; Calder, J.A. <i>Geochim. Cosmochim. Acta</i> <u>1976</u> , 40, 555-61.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of naphthalene in wate be 31.3 mg(1)/kg(2) and 2.43 x 10^{-4} m	$nol(1) dm^{-3}(2)$.	
The corresponding mass percent and moby the compiler are 3.13×10^{-3} g(1)/		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution 100 mL, was extracted with hexane, Concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	analytical grade; used as received; no impurities by	

ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.4 mg(1)/kg(2) (from eight determinations)

REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Water; H ₂ O; [7732-18-5]	Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.4-31.8°C	A. Maczynski

EXPERIMENTAL VALUES:

	Solubility of naphthalene in water		
t/°C	10 ⁴ mol(1) L ⁻¹	10 ³ g(1)/100 g sln (compiler)	$10^{6}x_{1}$ (compiler)
8.4	1.40 ± 0.02	1.79	2.52
11.1	1.49 ± 0.03	1.91	2.68
14.0	1.66 ± 0.05	2.13	2.99
17.5	1.88 ± 0.03	2.41	3.39
20.2	2.07 ± 0.02	2.65	3.73
23.2	2.22 ± 0.03	2.85	4.00
25.0	2.36 ± 0.02	3.03	4.25
26.3	2.48 ± 0.02	3.18	4.47
29.2	2.68 ± 0.02	3.44	4.83
31.8	2.83 ± 0.02	3.63	5.10

Two methods were used. (1 At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	DURCE AND PURITY OF MATERIALS:
At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	
dry and placed in the fluorimeter. so	 source not specified; better than 99.9 mole%, by glc; used as received. distilled over KMnO₄ and NaOH and passed through a Sephadex column. STIMATED ERROR: emp. ± 0.1°C
REI	oly. see above
	EFERENCES :

Components:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Schwarz, F.P.; Wasik, S.P.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 270-3.
VARIABLES:	PREPARED BY:
Temperature: 12-25°C	A. Maczynski
EXPERIMENTAL VALUES:	l
Solubility of naph	
t/°C 10 ⁴ mol(1) L ⁻¹	$\frac{10^3 \text{ g(l)/100 g sln} \qquad 10^6 x_1}{(\text{compiler})} \qquad (\text{compiler})$
12 1.57	2.01 2.83
18 1.90	2.43 3.42
25 2.34	3.00 4.21
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.	 (1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%. (2) distilled from KMnO₄ and passed through a Sephadex column. ESTIMATED ERROR: temp. ±0.1°C soly. ±2 x 10 ⁻⁶ mol(1) dm ⁻³
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of naphthalene in wate	er at 25°C was reported to be
31.69 mg(1)/kg(2).	
The corresponding mass percent and mo	
by compiler are 0.003169 g(1)/100 g s	$\sin and 4.425 \times 10^{-1}$.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The dynamic coupled column liquid	(1) commercial product; less than 3% impurities.
chromatography (DCCLC) method was based on generating saturated solu-	-
tions by pumping water through a column packed with glass beads that	(2) distilled over KMnO ₄ and NaOH and passed through a column
have been coated with the component (1) (generator column). The con-	packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).
centration of (1) in the effluent of the generator column was mea-	
sured by a modification of the	
coupled column liquid chromato- graphic process that has been de-	ESTIMATED ERROR:
scribed in ref 1.	temp. ± 0.05°C
	soly. ± 0.23 mg(1)/100 kg(2) (standard deviation)
	REFERENCES :
	 May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.;
	Dyszel, S. J. Chromatogr. Sci.
	<u>1975</u> , <i>13</i> , 535.

COMPONENTS:	EVALUATOR:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of naphthalene (1) in seawater (2) has been reported in six works:

Authors		Method	т/к	Salinity g salts/kg sln	10 ³ g(1)/100 g sln
Paul (ref l)	uv	spectral	298	30.59	2.53
Gordon and Thorne (ref 2)	uv	spectral	298	35.0	2.36
Gordon and Thorne (ref 3)	uv	spectral	298	31.7	2.47
Eganhouse and Calder (ref 4)		GLC	298	35	2.20
Schwarz (ref 5)	uv	spectral	298	30	2.17
May et al. (ref 6)		HPLC	298	35.0	2.29

At 298 K and a salinity of 35 g salts/kg sln the data of Gordon and Thorne (ref 2), Eganhouse and Calder, and May *et al.* are in good agreement. Therefore the mean value, 2.29×10^{-3} , is adopted as the recommended value at this temperature and salinity. Since the value of Schwarz is lower than would be expected with decreasing salinity, it is considered doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul and of Gordon and Thorne (ref 3) are in fair agreement. Therefore their mean is adopted as a tentative value. Gordon and Thorne (ref 2) and May *et al.* report data for a range of salinities using the Setschenow equation. Schwarz reports data over the temperature range 281 to 303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

	SOLUBILITY OF NAPHTHALENE (1) IN SEAWATER RECOMMENDED(r) AND TENTATIVE(t) VALUES	(2)
т/к	g salts/kg sln	10 ³ g(l)/100 g sln
298	<u>35 (r)</u>	2.29
298	31 (t)	2.5

REFERENCES

- 1. Paul, M.A. J. Amer. Chem. Soc. 1952, 74, 5274-7.
- 2. Gordon, J.E.; Thorne, R.L. J. Phys. Chem. 1967, 71, 4390-9.
- 3. Gordon, J.E.; Thorne, R.L. Geochim. Cosmochim. Acta 1967, 31, 2433-43.
- Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 5. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 6. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

HWW 2-R

	PREPARED BI:
e: 25°C	M. Kleinschmidt
64 g(3)/kg sln	
25:	
ubility of Naphthalene	in Aqueous Sodium
g(2)/kg sln [*] 10 ⁴ g-m	ol(1)/L ⁻¹ 10 ³ Ma
12.40 2.	37 3.0
25.31 2.	
30.59 2.	
43.70 1.	68 2.0
61.63 1.	38 1.6
by compilers using dens ons from ref l.	ity and other phy

DDEDADED DV VARIABLES: One temperature t and W. Shiu Salinity: 13-EXPERIMENTAL VALUE Sol m Chloride 10⁶ ×1^{*} $g-mol(3)/L^{-1}$ iss * 0.214 0.440 1 4.27 3.61 3 0.535 3.64 0.771 3.02 59 1.101 2.48

ORIGINAL MEASUREMENTS:

J. Am. Chem. Soc. 1952, 74,

Paul, M.A.

5274-7.

*Calculated k sical data for NaCl solution

AUXILIARY INFORMATION	
AUXILIARY METHOD/APPARATUS/PROCEDURE: Equilibration flask: 50-mL glass- stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until ex- cess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically con- trolled at 25.00 ± 0.05°C for at least 48 hr, and shaken occasionally during that time. Samples were with- drawn with a l0-ml transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultra-violet region of the spectrum.	<pre>SOURCE AND PURITY OF MATERIALS: (1) recrystallized from menthanol (2) reagent grade, dried at 120°C before weighing (3) redistilled Sources not specified.</pre>
	REFERENCES: 1. Weast, R.C.; CRC Handbook of Chemistry and Physics, 59th Edition; CRC Press <u>1978</u> , pp D299-D300.

COMPONENTS:

(1) Naphthalene; C₁₀H₈; [91-20-3]

(2) Sodium chloride; NaCl; [7732-14-5]

(3) Water; H₂O; [7647-18-5]

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Gordon, J.E.; Thorne, R.L.	
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Phys. Chem. <u>1967</u> , 71, 4390-9.	
(3) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 24.91°C Salinity: 0-108 g(2)/kg sln	M. Kleinschmidt and D. Shaw	
EXPERIMENTAL VALUES:		
The solubility of naphthalene in aque	ous sodium chloride is reported	
in terms of the Setschenow equation:	$\log(S_{o}^{S}) = K_{s}C_{s}$	
where, S _o is the solubility of naphthalene in water (mol/L) S is the solubility of naphthalene in solution (mol/L) K _s is the Setschenow constant (L/mol) C _s is the concentration of sodium chloride (mol/L)		
evaluating the equation for S over the range of C _S 0-2 mol/L, log S ₀ = -3.590 \pm 0.004 (95% confidence limit) and K _S = 0.220 \pm 0.0041 (95% confidence limit).		
The corresponding mass percent and mole fraction, x_1 at salinity = 35 g(2)/kg sln calculated by the compilers are 2.36 x 10 ⁻³ g(1)/100 g sln and 3.48 x 10 ⁻⁶ assuming a solution density of 1.025 kg/L.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Saturated solutions were prepared by equilibrating excess (1) in salt water in sealed ampols for 24 hrs. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.	 (1) recrystallized four times and sublimed or zone refined, 99.99+% pure, (2) analytical reagent grade, (3) distilled from potassium per- manganate and redistilled from all glass still. ESTIMATED ERROR: temp. ± 0.03°C solv. son above 	
	soly. see above REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Gordon, J.E.; Thorne, R.L.
(2) natural seawater	Geochim. Cosmochim. Acta, <u>1967</u> , 31, 2433-43.
VARIABLES:	PREPARED BY:
One temperature: 25°C	W.Y. Shiu and D. Mackay
Salinity: 10-32 g/kg sln	

Salinity ^b g/kg_sln	Chlorosity (°/)	Treatment ^a	log S <u>Observe</u> d	10 ⁴ s ^b g-mol(1)/ dm ³	10 ³ mass ratio ^b g(1)/100 g sln	10 ⁶ mole ₁ fraction X 1
31.8	17.96	MF	-3.715	1.93	2.47	3.47
			-3.717	1.92	2.46	3.45
31.8	17.96	GFF	-3.713	1.94	2.48	3.49
			-3.712	1.94	2.49	3.49
31.9	18.00	CENT	-3.704	1.98	2.53	3.56
ļ			-3.708	1.96	2.51	3.53
31.5	17.81	MF	-3.721	1.90	2.44	3.42
1			-3.722	1.91	2.45	3.41
31.8	17.95	GFF	-3.719	1.90	2.43	3.44
			-3.722	1.91	2.45	3.41
31.7	17.72	MF	-3.715	1.93	2.47	3.45
			-3.716	1.92	2.465	3.46
31.5	17.80	GFF	-3.719	1.91	2.45	3.41
1			-3.720	1.905	2.44	3.43
9.8	5.45	MF	-3.630	2.344	3.005	4.22
			-3.630	2.344	3.005 (continued	4.22)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Naphthalene: 99.99 + % from James Detail given in reference (1). Saturated solutions were prepared Hinton, Valparaiso, by equilibrating excess naphthalene Florida and salt solution in an ampoule with Salts: Analytical reagent grade shaking for 24 hours. The filtered from Mallinckrodt saturated solution was analyzed by Natural Seawater: collected at a UV Spectrophotometer. West Falmouth, Buzzards Bay, Quicks Hole and Mashapaquit Creek, Massachusetts ESTIMATED ERROR: Solubility ± 3% (Authors) Temperature ± 0.03°C (Authors) **REFERENCES:** Gordon, J.E.; Thorne, R.L. J. Phys. Chem. <u>1967</u>, 71, 4390. 1.

COMPONENTS:

(1) Naphthalene; C₁₀^{II}₈; [91-20-3]

(2) natural seawater

ORIGINAL MEASUREMENTS:

Gordon, J.E.; Thorne, R.L.

Geochim. Cosmochim. Acta <u>1967</u>, 31, 2433-43.

Experimental Values: (continued)

Salinity ^b g/kg sln	Chlorosity (°/)	<u>Treatment</u> ^a	log S Observed	10 [*] s ^b . g-mol(1)/ dm ³	l0³ mass ratio ^b g(l)/l00 q sln	10 ⁶ mole _b fraction X 1
9.8	5.45	GFF	-3.629	2.35	3.01	4.23
			-3.632	2.33	2.99	4.20

^aMF, membrane (0.45µ) filtered; GFF, glass fiber filtered; CENT, centrifuged

 $^{\rm b}$ Values calculated by compiler.

Temperature = 24.91°C

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ [91-20-3]	Eganhouse, R.P.; Calder, J.A.
(2) Artificial seawater (ref 1)	Geochim. Cosmochim. Acta <u>1976</u> , 40 555-61.
VARIABLES: One temperature: 25.0°C	PREPARED BY:
Salinity: 35 g/kg sln	M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES:	
The solubility of naphthalene in sea	water is reported to be
22.0 mg/kg sln. The corresponding m	ass percent and mole fraction,
x_1 , calculated by the compilers are 3.18 x 10 ⁻⁶ .	$2.20 \times 10^{-3} g(1)/100 g sln and$
Graphical results for other saliniti	es are also reported.
-	-
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	(1) analytical grade salts for
Equilibrium flask: 1 L Erlen- meyer flask with ground glass stopper and sidearm tap at base	(1) analytical grade saits for artificial seawater solution, reagent grade.
plugged with glass wool. The mixtures were agitated 12+ hr at	water: doubly distilled
215 rpm on a New Brunswick gyrotary shaker; a 24 hr station-	
ary equilibrium period followed.	
Hydrocarbons were extracted with doubly-distilled hexane 3 times;	
concentrated by evaporation, with	
losses checked against an internal standard.	ESTIMATED ERROR:
Standard.	temperature: ± 0.5°C
Analysis: gas chromatography	-
	soly: ± 0.293 (95% confidence interval).
	REFERENCES:
	 Lyman, J.; Fleming, R.H.; J. Mar. Res. <u>1940</u>, 3, 135.
	1

256	38_202
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	Schwarz, F.P.
(2) Sodium chloride; NaCl; [7647-14-5]	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 8.6-31.8°C	N Y Shin D Mackay
Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay
EXPERIMENTAL VALUES:	
Solubility of naphthalene	in 0.5 g-mol(2)/dm ³
	10 ⁴ mol(1)/L sln
8.6	0.84
11.1	0.92
14.0	1.09 1.23
20.0	1.37
23.0	1.58
25.0 31.8	1.73 2.22
3.13×10^{-6} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of naphthalene in NaCl	Naphthalene: purity > 99 mole %
solution was determined by fluores-	
cence and UV absorption measurements.	Sodium chloride: reagent grade
In the fluorescence method, saturated solution was prepared by adding	
excess amount of naphthalene to an	Water: distilled over a KMnO4 -
air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution.	NaOH solution and passed
The cell was rotated at 20 rpm for	through a Sephadex column.
at least 72 hr in a thermostatted water bath and then its fluorescent	
intensity was measured at 350 and	ESTIMATED ERROR:
315 nm. The Spectrofluorimeter em- ployed a ratio-photon counting mode	
where naphthalene concentration was	Solubility ± 3.3% (author)
linearly related to the fluorescence signal. The UV method was used to	Temperature ± 0.1°C (author)
obtain the absorptivity of naphtha-	REFERENCES:
lene in ethanol therefore provide an absolute solubility scale for the	
fluorescence method.	

38_203	257
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C ₁₀ H ₈ ; [91-20-3]	May, W.E.; Wasik, S.P.; Freeman D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
	cour rodium chlorido in
The solubility of naphthalene in aqu	
reported in terms of the Setschenow	equation:
$\log(S_0/S) = K_SC_S$	
where;	
S _o is the solubility	of (l) in water (mg/L)
S is the solubility o	f (l) in saline solution (mg/L)
K_{s} is the Setschenow	constant (L/mol)
$C_{_{\mathbf{S}}}$ in the concentrati	on of sodium chloride (mol/L)
evaluating the equation for S over t	he range of C _S 0-0.7 mol/L,
$K_{s} = 0.213$ with $S_{o} = 31.69$.	-
and 3.29 x 10^{-6} .	pilers are 2.29 x 10 ⁻³ g(l)/100 g sln
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water- acetonitrile solvent was passed through for extraction. The extract was introduced into a	(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.
liquid chromatograph and the concen- tration of (1) was measured with a UV detector.	ESTIMATED ERROR: temp \pm 0.05°C K _s \pm 0.001 S _o \pm 0.23
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) 1,2,4,5-Tetramethylbenzene; C₁₀H₁₄; [95-93-2] (2) Water; H₂O; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-244.			
VARIABLES:	PREPARED BY:			
One temperature: 25°C	M.C. Haulait-Pirson			
	-			
EXPERIMENTAL VALUES:	-			
The solubility of 1,2,4,5-tetramethylbenzene in water at 25°C and at				
system pressure was reported to be 3.	48 mg(1)/kg(2). The corresponding			
mass per cent and mole fraction, x_1 ,	calculated by the compiler are			

-	-			-					
mass	per	cent	and m	ole	fraction,	x,,	calculated	by the	compi
3.48	x 1	0 ⁻⁴ a	(1)/10)0 a	sln and 4	.67	$\times 10^{-7}$.		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were car- ried out using a Hewlett-Packard Model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	 Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. Distilled.
	ESTIMATED ERROR:
	Temperature: ±1°C
	Solubility: ±0.28 mg(l)/kg(2)
	REFERENCES :

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1,2,4,5-Tetramethylbenzene;</pre>	Krzyzanowska, T.; Szeliga, J.
C ₁₀ H ₁₄ ; [95-93-2]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4,5-tetramethylbenzene in water at 25°C was reported to be 3.48 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 3.48 x 10^{-4} g(1)/100 g sln and 4.67 x 10^{-7} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat- ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Sat- urated solutions of heptane in (2) were used as standard solutions.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.

COMPONENTS :	EVALUATOR:		
<pre>(1) p-Cymene; C₁₀H₁₄; [99-87-5] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.		

CRITICAL EVALUATION:

Quantitative solubility data for the p-cymene (1) - water (2) system have been reported in the publications listed in Table 1.

					Studies of
the p-	Cymene	(1) -	Water	(2) Sy	ystem

Reference	<i>т/</i> к	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin <i>et al</i> . (ref 2)	283-303	(2) in (1)	analytical
Banerjee <i>et al</i> . (ref 3)	298	(l) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF p-CYMENE (1) IN WATER (2)

Only two solubility values are available, both at 298K, but they are in poor agreement. The value of 0.04g(1)/100g sln reported by Booth and Everson (ref 1) is more than an order of magnitude greater than the value of 2.34 x 10^{-3} g(1)/100g sln reported by Banerjee *et al.* (ref 3). On the basis of comparison with similar systems the value of Banerjee *et al.* is more realistic.

2. SOLUBILITY OF WATER (2) IN p-CYMENE (1)

Only the values of Englin *et al*. (ref 2) are available and so no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al*. are generally reliable at T < 300K but somewhat high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

REFERENCES

- 1. Booth, H.S.; Everson, H.E. Ind. Eng. Chem. 1948, 40, 1491-3.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u>, 14, 1227-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-5]	Booth, H.S.; Everson, H.E.
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of p-cymene in water	r at 25°C was reported to
be 0.04 g(1)/100 mL(2). Assuming	a solution density of 1.00, the mass
Percentage and mole fraction, x_1 ,	calculated by the compilers are
0.04 g(1)/100 g sln and 5 x 10^{-5} .	
5	

AUXILIARY INFORMATION					
METHOD/APPARATUS/PROCEDURE: Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes and then centrifuged for 5 minutes. After this treatment, the volume of residue was determined directly.	<pre>Source AND PURITY OF MATERIALS: (1) source not specified; CP or highest commercial grade; used as received. (2) distilled. (2) distilled. ESTIMATED ERROR: soly. ± 0.1 mL(1)/100 mL(2). REFERENCES:</pre>				

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-6]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wa	ater in p-Cymene
<u>t/°C</u> g(2)/100 g sl	$\frac{10^3 x_2 (compiler)}{10^3 x_2 (compiler)}$
10 0.0223	1.66
20 0.0305 30 0.0415	2.27 3.08
AUXILIARY	INFORMATION
METHOD /AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	NOT Specified.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1)	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	G.T. Hefter		

EXPERIMENTAL VALUES:

METHOD/APPARATUS/PROCEDURE:

The solubility of p-cymene in water was reported to be 1.74 x 10^{-4} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1 , solubilities, calculated by the compiler, are 2.34 x 10^{-3} g(1)/100 g sln and 3.13 x 10^{-6} respectively.

AUXILIARY INFORMATION

Experiments were performed in sealed (1) Aldrich; purity not specified. stainless steel centrifuge tubes. An (2) Distilled. excess of p-cymene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete with in 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solu-ESTIMATED ERROR: tion were removed for analysis by GC after exhaustive extraction with hexane. A HP 5370A (FID) instrument and a 3% OV-1 on Chromosorb W column was used. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

ing one std. dev.)

SOURCE AND PURITY OF MATERIALS:

±0.2°C Temperature: ±3.1% rel. (represent-

So]	Lubi	111	:у:	

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Diethylbenzene; C ₁₀ H ₁₄ ; [25340-17-4]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility (iso	of Water in Diethylbenzene mer not specified)
<u>t/°C</u> <u>g(2)/100</u>	g sln $10^3 x_2$ (compiler)
$\begin{array}{ccccc} 0 & 0.01 \\ 10 & 0.02 \\ 20 & 0.03 \\ 30 & 0.04 \\ 40 & 0.05 \\ 50 & 0.07 \end{array}$	26 2.23 19 3.15 31 4.25 74 5.65
	AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced thermostatted flask and satur for 5 hr. with (2). Next, ca hydride was added and the evo hydrogen volume measured and 1 the concentration of (2) in (evaluated.	ated lcium (2) Not specified. lving hence
	ESTIMATED ERROR: Not specified.
	REFERENCES:

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COMPONENTS :	EVALUATOR:	
(1) <i>tert</i> -Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. A. Maczynski, Institute of Physical	
(2) Water; H ₂ O; [7732-18-5]	Chemistry, Polish Academy of Sciences Warszawa, Poland	
	February 1986.	

CRITICAL EVALUATION:

Quantitative solubility data for the tert-butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the tert-Butylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Englin et al. (ref 2)	283-303	(2) in (1)	analytical
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF TERT-BUTYLBENZENE (1) IN WATER (2)

The two reported solubilities of tert-butylbenzene in water are in reasonable agreement (Table 2).

TABLE		Tentative					
of	teri	t-Butylbenz	zene (1	.) i	n Wa	ter	(2)

T/K	Solubility values				
	Reported values	"Best" value ($\pm \sigma_n$) ^a			
	10 ³ g(1)/100g sln	10 ³ g(1)/100g sln 10 ⁶ x ₁			
298	3.4 (ref 1), 2.95 (ref 3)	3.2 ± 0.2 4.3			

a Obtained by averaging, σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN TERT-BUTYLBENZENE (1)

As only the solubility values of Englin *et al*. (ref 2) are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al*. are generally reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

(continued next page)

COMPONENTS: (1) tert-Butylbenzene; C₁₀H₁₄; [98-06-6] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Andrews, L.J.; Keefer, T.M. J. Am. Chem. Soc. 1950, 72, 5034-7.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.

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COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) tert-Butylbenzene; C₁₀H₁₄; [98-06-6]</pre> (2) Water; H ₂ O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.		
VARIABLES:			
VARIADLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
The corresponding mole fraction, x_1 is 4.6 x 10^{-6} .	calculated by the compilers		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophoto-	 (1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 167.8-168.0°C. (2) not specified. 		
meter.	LUIINILU LARVA.		
	not specified.		

REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) tert-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.		
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
VARIABLES:	PREPARED BY:		
Temperature: 10-30°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
Solubility of Water i	n tert-Butylbenzene		
$t/^{\circ}C$ g(2)/100 g sln	$10^3 x_2$ (compiler)		
10 0.0205 20 0.0292 30 0.0389	2.03 2.88 3.83		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.		
for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence	(2) Not specified.		
the concentration of (2) in (1) was evaluated.			
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) tert-Butylbenzene; C ₁₀ H ₁₄ ;	Sutton, C.; Calder, J.A.		
[98-06-5]	J. Chem. Eng. Data 1975, 20, 320-2.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
The solubility of tert-butylbenzene :	in water at 25°C was reported to be		
29.5 mg(l)/kg(2). The corresponding mass percent and mole fraction,			
x_1 , calculated by the compilers are 0.00295 g(l)/100 g sln and			
3.95×10^{-6} .			

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) tert-Butylbenzene; C₁₀H₁₄;</pre>	Sutton, C.; Calder, J.A.		
[98-06-6]	J. Chem. Eng. Data 1975, 20, 320-2.		
(2) Artificial seawater (ref 1)			
VARIABLES:	PREPARED BY:		
One temperature: 25.0°C			
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt and W. Shiu		
EXPERIMENTAL VALUES:			
The solubility of tert-butylbenzene :	in artificial seawater is reported to		
be 21.2 mg(l)/kg sln. The correspond	ling mass percent and mole fraction,		
x_1 calculated by the compiler are 2.	$12 \times 10^{-3} g(1)/100 g sln and$		
2.92 x 10^{-6} assuming the artificial s			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A test tube containing (1) was	(1) from either Aldrich Chemical		
placed in a flask containing (2) thus allowing for equilibration	Co. or Matheson Coleman and Bell, 99+% pure.		
through the vapor phase. The saturated solution was extracted	(2) made from doubly distilled		
with hexane and analyzed by gas	water and salts 99+% pure.		
chromatography.			
	ESTIMATED ERROR:		
	temp. ± 0.1°C		
	soly. 0.3 (std. dev.)		
	REFERENCES:		
	1. Lyman, J.; Fleming, R.H.;		
	J. Mar. Res. <u>1940</u> , 3, 135.		
	1		

COMPONENTS:		EVALUATOR -		
		EVALUATOR:		
<pre>(1) sec-Butylbenzene; C₁₀H₁₄; [135-98-8]</pre> (2) Water; H ₂ O; [7732-18-5]		A. Maczynski Institute of Physical Chemistry of the Polish Academy of Sciences Warszawa, Poland.		
-		November 1981		
 CRITICAL EVALUATION:				
The solubility of sec-butylbenzene (1) in water (2) has been reported in three works listed below:				
Authors	Method	T/K g(l)/100 g sln		
Andrews and Keefer (ref 1)	spectrophoto- 298.15 0.0309 metric			
Sutton and Calder (ref 3)				
Krzyzanowska and Szeliga (ref 4)	GLC	298.15 0.00101		
The data of Andrews and Kee remaining data is tentative		o be high. The mean value of the		
The solubility of water (2) one work listed below:	in sec-bu	tylbenzene (1) has been reported in		
Authors	Method	т/к		
Englin et al. (ref 2)	gasometr	ic 273.15-323.15		
Since these data are from o	one source	only, they are regarded as tentative.		
SOLUBILITY OF sec-BUTYLBENZENE (1) IN WATER (2) TENTATIVE VALUE				
SOLUBILITY OF se				
SOLUBILITY OF se		VALUE		
	TENTATIVE	$\frac{\text{VALUE}}{\text{g sln}} \qquad \frac{x_1}{-6}$		
<u>т/к</u> 298	<u>g(1)/100</u> 0.00	$\frac{\text{VALUE}}{\text{g sln}} \frac{x_1}{1.9 \times 10^{-6}}$		
<u>т/к</u> 298	<u>g(1)/100</u> 0.00	$\frac{\text{VALUE}}{\text{g sln}} \frac{x_1}{1.9 \times 10^{-6}}$ sec-BUTYLBENZENE (1)		
T/K 298 SOLUBILITY OF WA	<u>g(l)/l00</u> g(l)/l00 0.00 ATER (2) IN TENTATIVE	$\frac{\text{VALUE}}{\text{g sln}} \frac{x_1}{1.9 \times 10^{-6}}$ $\frac{\text{sec-BUTYLBENZENE (1)}}{\text{VALUES}}$		
<u>т/к</u> 298	<u>TENTATIVE</u> <u>g(l)/100</u> 0.00 ATER (2) IN	VALUEg sln x_1 141.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1)VALUESg sln x_2		
T/K 298 SOLUBILITY OF WA	<u>TENTATIVE</u> <u>g(1)/100</u> 0.00 ATER (2) IN <u>TENTATIVE</u> <u>g(2)/100</u> 0.02	VALUEg sln $\frac{x_1}{1}$ 141.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1)VALUESg sln $\frac{x_2}{0}$ 00.0020		
T/K 298 SOLUBILITY OF WA T/K 283 293	<u>TENTATIVE</u> <u>g(1)/100</u> 0.00 <u>ATER (2) IN</u> <u>TENTATIVE</u> <u>g(2)/100</u> 0.02 0.02	VALUEg sln x_1 141.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1)VALUESg sln x_2 00.002090.0029		
T/K 298 <u>SOLUBILITY OF WA</u> <u>T/K</u> 283 293 303	<u>TENTATIVE</u> <u>g(1)/100</u> 0.00 ATER (2) IN <u>TENTATIVE</u> <u>g(2)/100</u> 0.02	VALUEg sln x_1 141.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1)VALUESg sln x_2 00.002000.0029		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES	<u>TENTATIVE</u> <u>g(1)/100</u> 0.00 <u>ATER (2) IN</u> <u>TENTATIVE</u> <u>g(2)/100</u> 0.02 0.02 0.03	VALUEg sln $\frac{x_1}{1}$ 141.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1)VALUESg sln $\frac{x_2}{2}$ 00.002000.002900.0038		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A.	TENTATIVE g(1)/100 0.00 ATER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu	$yalue x_1 g sln x_1 14 1.9 x 10-6 sec-BUTYLBENZENE (1) VALUES g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. $		
T/K 298 SOLUBILITY OF WA 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma	TENTATIVE g(1)/100 0.00 ATER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965,	$yalue x_1 g sln x_1 14 1.9 x 10-6 sec-BUTYLBENZENE (1) VALUES g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. $		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	yalue g sln x_1 14 1.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1) yalues g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. eng. Data 1975, 20, 320-2.		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	$yalue x_1 g sln x_1 14 1.9 x 10-6 sec-BUTYLBENZENE (1) VALUES g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. $		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	yalue g sln x_1 14 1.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1) yalues g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. eng. Data 1975, 20, 320-2.		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	yalue g sln x_1 14 1.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1) yalues g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. eng. Data 1975, 20, 320-2.		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	yalue g sln x_1 14 1.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1) yalues g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. eng. Data 1975, 20, 320-2.		
T/K 298 SOLUBILITY OF WA T/K 283 293 303 REFERENCES 1. Andrews, L.J.; Keefer, 2. Englin, B.A.; Plate, A. Khim. Tekhnol. Topl. Ma 3. Sutton, C.; Calder, J.A	TENTATIVE g(1)/100 0.00 TER (2) IN TENTATIVE g(2)/100 0.02 0.02 0.03 R.M. J. A F.; Tugolu usel 1965, J. Chem	yalue g sln x_1 14 1.9 x 10 ⁻⁶ sec-BUTYLBENZENE (1) yalues g sln x_2 0 0.0020 9 0.0029 9 0.0038 mer. Chem. Soc. 1950, 72, 5034-7. xov, V.M.; Pryanishnikova, M.A. 10, 42-6. eng. Data 1975, 20, 320-2.		

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) sec-Butylbenzene; C₁₀H₁₄; [135-98-8] (2) Water; H₂O; [7732-18-5]</pre>	Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	•
The solubility of sec-butylbenzene is reported to be 0.0309 g(1)/100 g slu The corresponding mole fraction, x_1 is 4.15 x 10 ⁻⁶ .	1.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.	 (1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 175.0-175.8°C. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

COMPONENTS :		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ; [135-98-8]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.	
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. i Masel <u>1965</u> , 10, 42-6.	
VARIABLES:	PREPARED BY:	
Temperature: 10-30°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of water	in sec-butylbenzene	
t/°C g(2)/100 g s	$\frac{x_2 \text{ (compiler)}}{x_2 \text{ (compiler)}}$	
10 0.0226		
20 0.0317	0.00313	
30 0.0426	0.00420	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Component (1) was introduced into a thermostatted flask and saturated	(1) not specified.	
for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ;	Sutton, C.; Calder, J.A.		
[135-98-8]	J. Chem. Eng. Data 1975, 20, 320-2.		
(2) Water; H ₂ O; [7732-18-5]	520-2.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
The solubility of sec-butylbenzene in	n water at 25°C was reported to be		
17.6 mg(l)/kg(2). The corresponding	mass percent and mole fraction,		
x_1 , calculated by the compilers are (0.00176 g(l)/100 g sln and		
2.36×10^{-6} .			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The concentration of (1) in (2)	(1) Aldrich Chemical Co. or		
was determined by gas chroma- tography.	Matheson Coleman and Bell 99+%.		
	(2) distilled.		
	ESTIMATED ERROR:		
	temp. ± 0.1°C		
	soly. 0.2 (the standard deviation of the mean for six replicates).		
	REFERENCES:		

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) sec-Butylbenzene; C ₁₀ H ₁₄ ;	Krzyzanowska, T.; Szeliga, J.	
[135-98-8]	Nafta (Katowice), <u>1978</u> , 12, 413-7.	
(2) Water; H ₂ O; [7732-18-5]		
2		
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of sec-butylbenzene in	n water at 25°C was reported	
to be 10.1 mg(1)/kg(2).		
The corresponding mass percent and mo	ble fraction, x_1 , calculated	
by compiler are 0.00101 g(1)/100 g sl	In and 1.36 x 10^{-6} .	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.	
First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted	(2) not specified.	
at 25°C. Second, the mixture of (1)		
and (2) as above was thermostatted at 70°C and then cooled to 25°C. The		
time required to obtain equilibrium was three weeks. The solubility of		
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-		
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:	
ionization detector was used. Sat- urated solutions of heptane in (2)	<pre>soly. 0.3 mg(l)/kg(2) (standard</pre>	
Were used as standard solutions.	deviation from 7-9 determinations).	

REFERENCES:

COMPONENTS:ORIGINAL MEASUREMENTS:(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 3(2) Artificial seawater (ref 1)PREPARED BY:VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg slnPREPARED BY: M. Kleinschmidt and W. ShiuEXPERIMENTAL VALUES: The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fra x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and 1.64 x 10 ⁻⁶ assuming the artificial seawater composition of ref 1.	
[135-98-8] (2) Artificial seawater (ref 1) VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln EXPERIMENTAL VALUES: The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fra x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
(2) Artificial seawater (ref 1) VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln M. Kleinschmidt and W. Shiu EXPERIMENTAL VALUES: The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fra x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg slnPREPARED BY: M. Kleinschmidt and W. ShiuEXPERIMENTAL VALUES:The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fra x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
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The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fra x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole frace x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole frace x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	
x_1 calculated by the compiler are 1.19 x 10 ⁻³ g(1)/100 g sln and	action,
1	
1 -	
1.04 x 10 assuming the artificial seawater composition of ref 1.	
1	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
A test tube containing (1) was (1) from either Aldrich Chemic	
placed in a flask containing (2) thus allowing for equilibration Co. or Matheson Coleman an Bell, 99+% pure.	d
through the vapor phase. The	. 1
saturated solution was extracted (2) made from doubly distilled water and salts 99+% pure.	
chromatography.	
	ļ
ESTIMATED ERROR:	
temp. ± 0.1°C	
soly. 0.2 (std. dev.)	
REFERENCES:	_
1. Lyman, J.; Fleming, R.H.;	
J. Mar. Res. <u>1940</u> , 3, 135	i. (

COMPONENTS: (1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the

Butylbenzene (1) - Water (2) System			
Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Klevens (ref 2)	298	(1) in (2)	spectrophotometric
Jones and Monk (ref 3)	298-308	(2) in (1)	radiotracer
Englin et al. (ref 4)	283-303	(2) in (1)	analytical
Massaldi and King (ref 5)	298	(1) in (2)	GLC
Sutton and Calder (ref 6)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF BUTYLBENZENE (1) IN WATER (2)

The available data on the solubility of butylbenzene in water, all at 298K, are summarized in Table 2. The agreement is very poor with the reported values differing by almost two orders of magnitude which makes critical evaluation difficult. Fortunately, an independent estimation of the solubility can be made by extrapolation of the solubilities of the lower n-alkylbenzenes as a function of side chain length. This extrapolation predicts a value of 1.7×10^{-3} g(1)/100g sln. This value is quite close to the experimental values of Massaldi and King (ref 5) and Sutton and Calder (ref 6), the average of which is therefore suggested as the Tentative solubility of butylbenzene in water. The values of Andrews and Keefer (ref 1) and Klevens (ref 2) are correspondingly rejected.

COMPONENTS: (1) Butylbenzene; C₁₀H₁₄; [104-51-8] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Solubility of Butylbenzene (1) in Water (2)

T/K Solubility values "Best" values $(\pm \sigma_n)^a$ Reported values 10³g(1)/100g sln $10^{6} x_{1}$ 10³g(1)/100g sln 0.126^{b} (ref 1), 4.9^{b} (ref 2) 1.5 ± 0.3^{c} 298 2.0 1.77 (ref 5), 1.18 (ref 6) a Obtained by averaging but see text; $\sigma_{\mathbf{n}}$ has no statistical significance. b Rejected data, see text. c Tentative value, see text. 2. SOLUBILITY OF WATER (2) IN BUTYLBENZENE (1) Although two publications report solubility data of water in butylbenzene, that of Jones and Monk (ref 3) is reported in v/v fractions and is thus excluded from consideration. The remaining data of Englin et al. (ref 4) cannot therefore be evaluated. However it may be noted that the values of Englin et al. are usually reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant data sheet for the experimental values. REFERENCES 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1950, 72, 5034-7. 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98. 3. Jones, J.R.; Monk, C.B. J. Chem. Soc. 1963, 2633-5. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6. 4. 5. Massaldi, H.A.; King, C.J. J. Chem. Eng. Data 1973, 18, 393-7. 6. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. 1950, 72, 5034-7.
VARIABLES :	
One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in wat to be 0.000126 g(l)/100 g sln.	er at 25°C was reported
The corresponding mole fraction, x_1 , is 1.69 x 10 ⁻⁷ .	calculated by the compilers
15 1.09 X 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated	(1) Eastman Kodak Co. best grade;
for twenty hours in a constant	fractionally distilled;
temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was	b.p. range 182.0-183.0°C.
withdrawn and extracted with a	(2) not specified.
measured volume of hexane (10-50 mL) by shaking in a glass-stoppered	
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas-	
ured against a hexane blank on the	
Beckman spectrophotometer.	
	ESTIMATED ERROR: Not specified.
	Not opcorriga.
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in wat	or at 25°C was reported to be
0.05 g(1) L^{-1} sln and 0.00037 mol(1)	
1.00 kg sln = 1.00 L sln the mass per	ccentage and mole fraction x_1
calculated by the compilers are 0.005	$5 g(1)/100 g sln and 6.7 x 10^{-6}.$
l	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was	(1) not specified.
determined by shaking small amounts of (1) in 1 liter of (2) for as long	(2) not specified.
as three months. Aliquots were removed and concentrations deter-	
mined by spectra.	
}	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Jones, J.R.; Monk, C.B.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1963</u> , 2633-35.
VARIABLES:	PREPARED BY:
Temperature: 25-35°C	A. Maczynski, Z. Maczynska and A. Szafranski

The solubility of water in butylbenzene

t/°C	10 ⁴ mL(2)/mL(1)
25	3.5
30	4.1
35	4.9

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a thermostatted glass-stoppered flask $10-25 \text{ mL}(1)$ was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mc/mL), decanted, a 5-mL aliquot reshaken for 4 hrs. with 5 mL H ₂ O in a $10-\text{mL}$ flask, sampled and as a sayed with a Nuclear Enter- prises type 8301 liquid scintilla- tion counter. The two-stage process eliminates quenching effects (due to solvent) on the scintillator.	 (1) laboratory grade dried over CaCl₂ and fractionally distilled. (2) not specified.
	ESTIMATED ERROR: soly. ± 5% to ± 1% (average deviation)
	REFERENCES: 1. Vogel Practical Organic Chemistry Longmans, Green and Co., London, <u>1956</u> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Butylbenzene; C₁₀H₁₄; [104-51-8] (2) Water; H₂O; [7732-18-5] VARIABLES: Temperature: 10-30°C</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6. PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Wate	•
$\frac{t/^{\circ}C}{g(2)/100 \text{ g sl}}$	$\frac{10^3 x_2 (\text{compiler})}{10^3 x_2 (\text{compiler})}$
10 0.0234 20 0.0331 30 0.0448	1.74 2.46 3.33
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) Not specified.(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:ORIGINAL MEASUREMENTS:(1) Butylbenzene; C10H14; [104-51-8]Massaldi, H.A.; King, C.J.(2) Water; H20; [7732-18-5]J. Chem. Eng. Data 1973, 18, 393-7.VARIABLES:PREPARED BY:One temperature: 25°CA. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:The solubility of butylbenzene in water at 25°C was reported to be1.32 x 10⁻⁴ mol(1) dm⁻³ sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00177 g(l)/100 g sln and 2.4 x 10^{-6} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A technique based on head-space analysis by gas-liquid chromato- graphy was developed to determine solubilities of sparingly soluble	SOURCE AND PURITY OF MATERIALS: (1) Matheson Coleman and Bell Co., highest purity; used as received.
organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is ver- satile enough to allow determina- tions provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.	(2) not specified.
	ESTIMATED ERROR: temp. ± 0.05°C
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in wat	er at 25°C was reported to be
<pre>11.8 mg(l)/kg(2). The corresponding</pre>	mass percent and mole fraction,
x_1 , calculated by the compilers are 0 1.58 x 10 ⁻⁶ .	.00118 g(l)/100 g sln and
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	 (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.1 mg(1)/kg(2) (the standard deviation of the
	mean for six replicates) REFERENCES:
1	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; C10H14; [104-51-8]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2
	9. onem. Eng. Dava <u>1979</u> , 20, 520 2
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES:	
The solubility of butylbenzene in ar	tificial seawater is reported to be
7.09 mg(l)/kg sln. The correspondin	-
	$09 \times 10^{-4} \text{ g(1)/kg sln and 9.76 x 10^{-7}$
assuming the artificial seawater com	position of ref 1.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A test tube containing (1) was	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical
placed in a flask containing (2)	Co. or Matheson Coleman and
thus allowing for equilibration through the vapor phase. The	Bell, 99+% pure.
saturated solution was extracted with hexane and analyzed by gas	(2) made from doubly distilled water and salts 99+% pure.
chromatography.	-
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.07 (std. dev.)
	REFERENCES:
	 Lyman, J.; Fleming, R.H.; J. Mar. Res. 1940, 3, 135.
	<u></u>

286			38_23
COMPONE	NTS:		ORIGINAL MEASUREMENTS:
	+) - (R) - P-Mentha d -Limonene) · C	a-1,8-diene 0 ^H 16; [5989-27-5]	Massaldi, H.A.; King, C.J.
	ater; H ₂ 0; [773		J. Chem. Eng. Data <u>1973</u> , 18, 393-7.
(2) 1		,2 10 5]	
VARIABL	PC -		
	rature: 0-25°C		PREPARED BY: A. Maczynski and Z. Maczynska
rempe			
EXPERIM	ENTAL VALUES:		
5	Sc	blubility of d-lim	onene in water
t/°C	mg(l) L sln	10 ⁴ mol(1) L sl	$10^3 g(1)/100 g sln$ (compiler) $10^6 x$
0	9.7	0.708	0.97 1.3
5	10.4	0.767	1.04 1.4
25	13.8	1.013	1.38 1.8
		AUXILIARY	INFORMATION
METHOD /	APPARATUS/PROCEDUR	E:	SOURCE AND PURITY OF MATERIALS:
	hnique based on sis by gas-liqu		 Matheson Coleman and Bell Co., highest purity; kept under N2
graph	y was developed ilities of spar	l to determine	atmosphere at -2°C in a dark container; used as received.
organ	ics. Saturated	solutions need	(2) not specified.
phase	separation pro		(2) not specified.
be an	alyzed. This make in a enough to all	nethod is ver-	
tions	provided that	the pure vapor	
The g Aerog			ESTIMATED ERROR: temp. ± 0.05°C
		ļ	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Bicyclo[4.4.0]decane (deca-	G.T. Hefter, School of Mathematical
hydronaphthalene; decalin); C ₁₀ H ₁₈ ; [91-17-8]	and Physical Sciences, Murdoch
	University, Perth, W.A., Australia.
(2) Water; H ₂ O; [7732-18-5]	
	April 1986.
	1

CRITICAL EVALUATION:

Quantitative solubility data for the decalin (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin et al. (ref 2)	293-313	(2) in (1)	analytical
Price (ref 3)	298	(1) in (2)	GLC

TABLE 1: Quantitative Solubility Studies of theDecalin (1) - Water (2) System

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DECALIN (1) IN WATER (2)

The solubility of decalin in water has been reported only at 298K (Table 1). However, the datum of Booth and Everson (ref 1) in v/v fraction, is only an order of magnitude result and must thus be excluded. Since this leaves only the single datum of 8.89 x $10^{-5}g(1)/100g \sin(x_1 = 1.16 \times 10^{-7})$ of Price (ref 3) no Critical Evaluation is possible. Nevertheless, it may be noted that the solubility values reported by Price are usually reliable although for the higher hydrocarbons his results are often about 20% (relative) lower than Recommended values.

2. SOLUBILITY OF WATER (2) IN DECALIN (1)

As only the data of Englin *et al*. (ref 2) over the range 293-313K are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al*. are generally reliable when T < 300K but are somewhat high at higher temperatures. The interested user is referred to the relevant data sheet for the experimental values.

REFERENCES

1.	Booth,	H.S.;	Everson, H.H	. Ind.	Eng.	Chem.	1948,	40	, 1491-3.
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- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 Bicyclo[4.4.0]decane (Decahydro- naphthalene); C₁₀H₁₈; [91-17-8] Water; H₂O; [7732-18-5] 	Booth, H.S.; Everson, H. Ind. Eng. Chem. <u>1948</u> , 4, 1491-3.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	G.T. Hefter		
EXPERIMENTAL VALUES:			
The solubility of bicyclo[4.4.0]decane in water at 25°C was reported to			
be <0.02 mL(1)/100 mL(2).			
A similar result was reported for (1) in 40.0% (w/w?) aqueous sodium			
xylenesulfonate.			

AUXILIARY	INFORM	ATION
METHOD/APPARATUS/PROCEDURE:	SOURCE	AND PURITY OF MATERIALS:
A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.03 mL. An excess of solute was added and the mixture allowed to come to equi- librium in a constant temperature bath then centrifuged. The amount	(1)	"Highest grade commercial sam- ple available"; no other details given.
		Distilled.
of solute dissolved was determined by subtracting the undissolved solute, measured directly in the		
tube, from the total added.	ESTIM	ATED ERROR:
	Not	specified.
	REFER	ENCES :

38_233	2
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bicyclo[4.4.0] decane (deca- hydronaphthalene; decalin) C ₁₀ H ₁₈ ; [91-17-8]	Englin, B.A.; Plate, A.F.; Tugoluko V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and M.C. Haulait-Pirso
EXPERIMENTAL VALUES:	
Solubility of Water i	n Bicyclo[4.4.0]decane
<u>t/°C</u> <u>g(2)/100</u>	$\frac{10^4 x_2}{(\text{compiler})}$
20 0.00	
30 0.01 40 0.01	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	(2) Not specified.
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bicyclo[4.4.0]decane (deca-	Price, L.C.
hydronaphthalene;decalin); C ₁₀ H ₁₈ ; [91-17-8]	Am. Assoc. Petrol. Geol. Bull.
(2) Water: H_0 : [7732-18-5]	<u>1976</u> , <i>60</i> , 213-44.

(2) Water; H₂O; [7732-18-5] VARIABLES: One temperature: 25°C M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of bicyclo[4.4.0]decane in water at 25°C and at system pressure was reported to be 0.889 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 8.89 x 10⁻⁵ g(l)/l00 g sln and 1.16 x 10⁻⁷.

AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	 (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1°C soly. ± 0.031 mg(1)/kg(2)
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Pentylcyclopentane; C₁₀H₂₀; [3741-00-2] (2) Water; H₂O; [7732-18-5]</pre>	Price, L.C. Am. Assoc. Petrol. Geol. Bull. <u>1976</u> , 60, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

The solubility of pentylcyclopentane in water at 25°C and at system pressure was reported to be 0.115 mg(l)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler was 1.15 x 10⁻⁵ g(l)/100 g sln and 1.5 x 10⁻⁸.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were car- ried out by GLC using a Hewlett- Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) Distilled.</pre>
	ESTIMATED ERROR: Temp. ±1°C Soly. ±0.011 mg(1)/kg(2) REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Decene; C ₁₀ H ₂₀ ; [872-05-9] (2) Water; H ₂ O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. J. Chem. Eng. Data. <u>1972</u> , 17, 328-9.
VARIABLES:	PREPARED BY:
Temperature: 15-25°C	M.C. Haulait-Pirson and G.T. Hefter

	Solubility of 1-decene	in 0.001 mol/L HNO ₃ sln.	
t/°C	10 ⁵ mol/L sln ^a g(l)/100 g sln	10 ³ g(1)/100 g sln ^b (compiler)	10 ⁶ x ₁ (compiler)
15	8.2	1.1	1.5
20	6.1	0.85	1.1
25	4.1	0.57	0.73

^a Uncertainties stated to be "standard deviations from mean".
 ^b Assuming a solution density of 1.00 g mL⁻¹ at all temperatures.

Compilers' note:

Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the olefin solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HC^g.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged) visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titra- tion with bromine using standard procedures.	(1) BDH: 99%(2) Not specified.
	ESTIMATED ERROR:
	Temp. ±0.05 K
	Soly. see Table above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2,7-Dimethyloctane; C ₁₀ H ₂₂ ; [1072-16-8]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.	
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.	
VARIABLES:	PREPARED BY:	
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of Water in 2,7-Dimethyloctane		

<u>t/°C</u>	g(2)/100 g sln	10 ⁴ x ₂ (compiler)
10	0.0048	3.79
20	0.0087	6.87
30	0.0152	12.00

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) Not specified.(2) Not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES :

COMPONENTS:	EVALUATOR:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Water; H ₂ O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	1

CRITICAL EVALUATION:

Quantitative solubility data for the decane (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	Т/К	Solubility	Method
Baker (ref 1,2)	298	(1) in (2)	radiotracer
Schatzberg (ref 3)	298,313	(2) in (1)	Karl Fischer
Franks (ref 4)	298	(1) in (2)	GLC
McAuliffe (ref 5)	298	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 7)	298	(1) in (2)	GLC
Mackay et al. (ref 8)	_ ^a	(1) in (2)	GLC
Namiot $et \ al.$ (ref 9)	423-583 ^b	(2) in (1)	<pre>vapliq.equil.</pre>
Skripka (ref 10)	398-563 ^b	(2) in (1)	<pre>vapliq.equil.</pre>
Becke and Quitzsch (ref 11)	293	mutual	refractometric

TABLE 1: Quantitative Solubility Studies ofthe Decane (1) - Water (2) System

a Not specified but probably 298.15K. b Pressure also varied 1-78 MPa.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition, Roof (ref 6) has reported a three phase critical point of unknown composition at 569K and 9.6 MPa. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DECANE (1) IN WATER (2)

The available data on the solubility of decane in water are summarized in Table 2 with the following exceptions. The value of Baker in ref 2 is quoted in v/v terms and is therefore excluded from consideration (however it is equivalent to that reported by the same author in ref 1). The values of Mackay *et al.* (ref 8) are rejected not only because the measurement temperature was unspecified but also because the authors themselves regard their solubility values below $2 \times 10^{-3}g(1)/100g$ sln as potentially unreliable because of emulsion or colloid formation. The value of McAuliffe (ref 5) is also rejected because it is very much higher than all other reported values.

Agreement among the remaining values (Table 2) is not good enough to enable any of the "Best" values to be Recommended.

(continued next page)

r			
COMPONENTS :		EVALUATOR:	
(1) Decane; C ₁₀	H ₂₂ ; [124-18-5]	M.C. Haulait-Pirson, Depart Chemistry, University of Lev	
(2) Water; H ₂ O;	[7732-18-5]	Belgium.	
2		G.T. Hefter, School of Mathe and Physical Sciences, Murde	och
		University, Perth, W.A., Au	stralia.
CRITICAL EVALUATION	(continued)		
	TABLE 2: Tentative Va Decane (1) 1	lues of the Solubility of Mater (2)	
т/к	Solu	bility values	
	Reported values	"Best" values	$(\pm \sigma_n)^{\alpha}$
	10 ⁶ g(1)/100g sln	"Best" values 10 ⁶ g(1)/100g sln	10 ⁹ x ₁
293 1.98	(ref 11)	2	2.5
	(ref 1), 1.98 (ref 4),	1.5 ± 0.5	1.9
	(ref 7)		
- <u> </u>			
a Obtained by a	veraging; o nas no sta	tistical significance.	
2. SOLUBILITY	OF WATER (2) IN DECANE	: (1)	
At atmospheric p	pressure the only avail	able values of the solubilit	y of
water in decane	are those of Schatzber	g (ref 3) and Becke and Quit	zsch
(ref 11). These	e data are listed in Ta	ble 3 but are in poor agreem	ent and
can only be rega	arded as order of magni	tude values.	
• • • • • •			
		ly the data of Skripka and c	
		tical Evaluation is possible	
interested user is referred to the relevant Data Sheets for the experiment- al values.			
TABLE 3: Approximate Solubility Values of			
	Water (2) in	Decane (1)	
 Т/К	Poporto	d values ^a	
	.0 ² g(2)/100g sln	$10^3 x_2$	
_		2	
293	2.92 (ref 11)	2.3	
298	0.72 (ref 3)	0.6	
313	1.36 (ref 3)	1.1	
α Values considered as order-of-magnitude data only, see text.			
REFERENCES			
	 Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u>, 3, No.4, C61-8. 		
	,, ,, , ,, , ,, , , , , , , , , , , , , , , , , , , ,		
3. Schatzberg,	P. J. Phys. Chem. 1		
·····	····	(continued ne:	xt page)

COMPONENTS: (1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂O; [7732-18-5] CRITICAL EVALUATION: (continued) EVALUATOR: M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

REFERENCES (continued)

4. Franks, F. Nature <u>1966</u>, 210, 87-8.

5. McAuliffe, C. Science 1969, 163, 478-9.

6. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3.

- Krasnoshchekova, P.Y.; Gubergrits, M.Y. Neftekhimiya <u>1973</u>, 13, 885-7.
- Mackay, D.; Shiu, M.W.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, <u>1975</u>, 251-8.
- 9. Namiot, A.Y.; Skripka, V.G.; Lotler, Y.G. Zh. Fiz. Khim. <u>1976</u>, 50, 2718; Deposited doc. 1976; VINITI 1213-76.
- 10. Skripka, V.G. Tr. Vses. Neftegazov. Nauch-Issled. Inst. <u>1976</u>, 61, 139-51.

11. Becke, A.; Quitzsch, G. Chem. Techn. 1977, 29, 49-51.

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38_239	297	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Baker, E.G.	
(2) Water; H ₂ O; [7732-18-5]	Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u> , 3, N°4, C61-8.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of decane-1-C ¹⁴ in water at 25°C was reported to be 16 x 10^{-9} g(1)/g(2). The corresponding mole fraction, calculated by the compiler, is $x_1 = 2.0 \times 10^{-9}$.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Carbon-14 labeled (1) was used as radioactive tracer. The technique of preparing a satu- rated aqueous solution of (1) by ultrafiltration of a (1)-(2) dis- persion has been described in ref 1. A Packard Tri-Carb Liquid Scintilla- tion Spectrometer was used to detect the radioactive (1) dissolved in (2).	(1) Nuclear Instrument and Chemical Corporation; used as received.(2) distilled.	
	ESTIMATED ERROR:	
	soly. 20% (standard deviation from 17 replicate runs).	
	REFERENCES :	
	 Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints- Symposia <u>1956</u>, 1, N°2, 5. 	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Science 1959, 129, 871-4.
_	
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of decane in water at $22 \times 10^{-7} \text{ mL}(1)/100 \text{ mL}(2)$.	25°C was reported to be
22×10 mL(1)/100 mL(2).	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
not specified.	not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wat	er in decame
	'kg sln x ₂
	<u> </u>
25	2^{a} 5.7 x 10 ⁻⁴
40 136	10.7×10^{-4}
a,b See "Estimated Error"	
See Estimated EITOP	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a	(1) Phillips Petroleum Co.; research
layer of (2) in a brown glass bottle	grade; 99.43 mole%; passed
without any agitation. The bottle was sealed with serum cap and com-	repeatedly through a column of silica gel until no absorp-
pletely submerged in the water-bath	tion occurred in the 220 to
for 7 days. A 20-mL sample was withdrawn with a silicone-hydro-	340 nm spectral range.
phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted	(2) distilled and deionized.
to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly	ESTIMATED ERROR:
in the presence of methanol to a	temp. ± 0.02°C
"dead-stop" end-point using a	
Beckman KF3 automatic titrimeter.	<pre>soly. a) 0-6%; b) 0-2% (deviations from the mean)</pre>
Beckman KF3 automatic titrimeter.	
Beckman KF3 automatic titrimeter.	from the mean)
Beckman KF3 automatic titrimeter.	from the mean)
Beckman KF3 automatic titrimeter.	from the mean)
Beckman KF3 automatic titrimeter.	from the mean)

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COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Franks, F.	
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1966</u> , 21 0, 87-8.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	F. Kapuku	
EXPERIMENTAL VALUES:	<u> </u>	
The solubility of decane in water at 25°C was reported to be in mole fraction $x_1 = 2.5 \times 10^{-9}$. The corresponding mass percent calculated by the compiler is 1.98 x 10 ⁻⁶ g(1)/100 g sln.		
AUXILIARY INFORMATION		

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 ml of the aqueous phase was injected into the fractionator fitted to the chroma- tographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.	<pre>(1) Fluka; purum grade; purity > 97% (chromatographic analysis). (2) not specified. ESTIMATED ERROR: soly. ± 12% REFERENCES:</pre>

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COMPONENTS:	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Science <u>1969</u> , 163, 478-9.
VADIANI DO .	
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of decane in water at	25°C was reported to be
0.052 mg(1)/kg(2).	
The corresponding mass percent and mo by the compiler are 5.2×10^{-6} g(1)/1	
by the compiler are 5.2 x 10 g(1)/1	oo g sin and 6.58 x 10 .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with (2). Glass vials were filled with the saturated	-
aqueous phase. Half of water was then displaced and replaced by air.	(2) distilled.
The vials were then sealed and shaken	
for 2 minutes. The gas phase was then displaced through the sample	
loop of a gas chromatograph for analyzing for hydrocarbon content.	
	ESTIMATED ERROR:
	soly. ± 0.0043 mg(1)/kg(2)
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.	
(2) Water; H ₂ O; [7732-18-5]		
_	Neftekhimiya <u>1973</u> , 13, 885 - 7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski	
-	-	
EXPERIMENTAL VALUES:		
The solubility of decane in water at 25°C was reported to be		
$x_1 = 1.1 \times 10^{-9}$.		
The corresponding mass percent calcu	lated by the compiler is	
$8.7 \times 10^{-7} g(1)/100 g sln.$		
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
A mixture of 10 mL (1) and 300 mL	(1) source not specified;	
(2) was placed in a double-walled	CP reagent; purity not	
bottom-stoppered vessel and vigor- ously stirred magnetically for 10-	specified.	
12 hr. The phases were allowed to	(2) distilled.	
separate; a first sample of the water phase was rejected and next		
200 mL of this phase was taken, 20-mL aliquots were introduced into		
40-mL hermetic bottles and (1) was		
allowed to equilibrate with the air, and the (1)-saturated air was		
analyzed by glc.	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Mackay, D.; Shiu, W.J.; Wolkoff, A.W.
(2) Water; H ₂ O; [7732-18-5]	"Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u> , <i>573</i> , 251-8.
VARIABLES:	PREPARED BY:
not specified	M.C. Haulait-Pirson

The authors reported two different values for the solubility of decane in water: 0.182 and 1.22 mg(1)dm⁻³ sln. With the assumption of a solution density of 1.00 g cm⁻³, the corresponding mass percents calculated by the compiler, are 0.0000182 and 0.000122 g(1)/100 g sln and the corresponding mole fractions, x_1 , are 2.3 x 10⁻⁸ and 1.6 x 10⁻⁷ respectively.

AUXILIARY INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equili- brations it is possible to calculate the amount of (1) in the original sample.	 (1) not specified. (2) not specified. ESTIMATED ERROR:	
	not estimated.	
	REFERENCES :	

COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]			Namiot, A.Yu.; Skripka, V.G.; Lotter, Yu.G.	
(2) Water; H ₂ O; [7732-18-5]		Zh. Fiz. Khim. <u>1976</u> , 50, 2718 <u>Deposited doc.</u> 1976, VINITI 1213-76.		
VARIABLES:			PREPARED BY:	-
	ure: 150-310°C : 0.52-8.44 MPa		A. Maczynski	
EXPERIMENTA	L VALUES:			
	Solub	ility of wat	er in decane	
t/°C	$p/kg \text{ cm}^{-2}$	p/MPa (compiler	., ^x 2	g(2)/100 g sln (compiler)
150	5.3	0.52	0.028	0.36
200 225	18.2	1.79 2.9	0.095 0.162	1.31 2.39
225	30 47.2	2.9 4.63		2.39 4.01
250	73.2	4.03	0.248	7.87
285	83.9	8.23	0.504	11.4
290	95.4	9.36	0.606	16.3
310	20	2.0	0.029	0.38
310	30	2.0	0.029	0.93
310	40	3.0	0.114	1.60
310	50	4.9	0.171	2.54
310	60	5.9	0.239	3.82
310	70	6.9	0.313	5.45
310	80	7.8	0.407	7.99
310	86.1	8.44	0.520	12.06
	· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFORMATION	
METHOD/APPA	RATUS/PROCEDURE:		SOURCE AND PURITY	OF MATERIALS:
equilibri	ic method for vap ium described in :			specified; CP used as received.
used. No more details were reported in the paper.		(2) distilled.		
			ESTIMATED ERROR:	
			not specified.	
			REFERENCES:	
			l. Sultanov, H	R.G.; Skripka, V.G.; A. Zh. Fiz. Khim. 2170.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Decane; C₁₀H₂₂; [124-18-5] (2) Water, H₂0; [7732-18-5]</pre>	 Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u>, 61, 139-51. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u>, 47, 1035.
VARIABLES:	PREPARED BY:
Temperature: 225-290°C Pressure: 2.9-78.5 MPa	A. Maczynski
EXPERIMENTAL VALUES: Solubility of wa	ter in decane
t/°C p/kg cm ⁻² p/MI	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.157 2.30 0.153 2.28 0.148 2.15 0.138 1.99 0.132 1.89 0.124 1.76 0.118 1.67 0.108 1.51 0.102 1.42 0.098 1.36 0.095 1.31
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccc} 0.248 & 4.01 \\ 0.240 & 3.84 \\ 0.226 & 3.56 \\ 0.213 & 3.31 \\ 0.200 & 3.07 \\ 0.190 & 2.88 \\ 0.168 & 2.49 \\ 0.158 & 2.32 \\ 0.153 & 2.24 \end{array}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The experimental technique was described in ref 1. No details reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified, chemical reagent grade; purity not specified; used as received. (2) distilled.</pre>
	ESTIMATED ERROR: not specified. REFERENCES: 1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. <u>1971</u> , 4, 6.

<pre>(1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂O; [7732-18-5]</pre>		Tr. Vses Inst. Sultanov	 Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. <u>1976</u>, 61, 139-51. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035. 		
t/°C	p/kg cm ⁻²	p/MPa (compiler)	*2	g(2)/100 g sln (compiler)	
275	70	6.9	0.404	7.90	
	100	9.8	0.385	7.34	
	150	14.7	0.353	6.46	
	200	19.6	0.320	5.62	
	250	24.5	0.293	4.98	
	300	29.4	0.272	4.52	
	400	39.2	0.246	3.97	
	500	49.0	0.231	3.66	
	600	58.8	0.217	3.39	
	700	68.6	0.204	3.14	
	800	78.5	0.197	3.08	
290	100	9.8	0.580	14.88	
	150	14.7	0.417	8.30	
	200	19.6	0.392	7.54	
	250	24.5	0.371	6.95	
	300	29.4	0.350	6.38	
	400	39.2	0.318	5.57	
	500	49.0	0.291	4.94	
	600	58.8	0.270	4.47	
	700	68.6	0.253	4.11	
	800	78.5	0.243	3.90	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Becke, A.; Quitzsch, G.		
(2) Water; H ₂ O; [7732-18-5]	Chem. Techn. <u>1977</u> , 29, 49-51.		
VARIABLES:	PREPARED BY:		
One temperature: 20°C	P.L. Huyskens and M.C. Haulait-Pirson		

The solubility of decane in water at 20°C was reported to be in mole fraction, $x_1 = 2.5 \times 10^{-9}$. The corresponding mass percent, calculated by the compiler, is 1.976 $\times 10^{-6}$ g(1)/100 g sln. The solubility of water in decane at 20°C was reported to be in mole fraction, $x_2 = 2.3 \times 10^{-3}$. The corresponding mass percent, calculated by the compiler, is 0.0292 g(2)/100 g sln.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The refractometric and the Karl- Fischer dead-stop titration methods were used. No more details are given in the paper.	not specified.		
	ESTIMATED ERROR:		
	soly. 0.05-1% for (1) in (2) 0.3-1.3% for (2) in (1)		
	REFERENCES:		

500			50_24
COMPONENTS :		EVALUATOR:	
 (1) Decane; C₁₀H₂₂; [124-18-5] (2) Seawater 		D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA	
		December 1982	
CRITICAL EVALUATION:	_		
The solubility of decane	(l) in seawa	ter (2) has been	reported in two
works:			
Authors	Method T/	Salinity K g salts/kg sl	n g(l)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC 29	8 6	8.7×10^{-6}
Freegarde <i>et al</i> . (ref 2)	GLC ?	?	1.5×10^{-5}
	DOUBTFUL		
т/к 	g salts/k		g(1)/100 g sln
298	6		8.7×10^{-6}
REFERENCES			
 Krasnoshchekova, R.Ya 13, 885-8. 	.; Gubergrit	s, M.Ya. Neftek	himiya <u>1973</u> ,
 Freegarde, M.; Hatcha 20, 35-40. 	rd, C.G.; Pa	cker, C.A. Lab.	Pract. <u>1971</u> ,

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Freegarde, M.; Hatchard, C.G.; Parker, C.A.
<pre>(2) Seawater (composition not specified)</pre>	Lab Pract. <u>1971</u> , 20, 35-40.
VARIABLES:	PREPARED BY:
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES:	■ · · · · · · · · · · · · · · · · ·
The solubility of decane was reported	d to be 0.15 mg/L. The
corresponding mass percent and mole :	-
the compilers are $1.5 \times 10^{-5} g(1)/100$	0 g sln and 1.9 x 10^{-8} ,
assuming a solution density of 1.02	kg/L.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
None given except that analysis was done using gas chromatography.	not given.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :
	ļ

310	38_251		
COMPONENTS: (1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater	ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885-8.		
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln	PREPARED BY: M. Kleinschmidt		
Salinity: 6 g/kg sln M. Kleinschmidt EXPERIMENTAL VALUES: The solubility of decane in seawater was reported to be 8.7 x 10^{-6} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 1.1 \times 10^{-8}$.			
AUVILLADY INFORMATION			

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solu- tion was then transferred to a closed flask with head space volume equal to solution volume. Hydro- carbon concentration in the head space was determined by gas chroma- tography and the corresponding	 (1) "chemically pure" (2) distilled water plus salt mixture.
solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES :
	KEFEKENCES:

38_2	52
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COMPONENTS:	EVALUATOR:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 1-methylnaphthalene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the1-Methylnaphthalene (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin et al. (ref l)	273-323	(2) in (1)	analytical
Eganhouse and Calder (ref 2)	298	(1) in (2)	GLC
Mackay and Shiu (ref 3)	298	(1) in (2)	spectrofluorometric
Schwarz and Wasik (ref 4)	283-298	(1) in (2)	spectrofluorometric
Schwarz (ref 5)	282-305	(1) in (2)	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For further convenience further discussion of this system is divided into two parts.

1. SOLUBILITY OF 1-METHYLNAPHTHALENE (1) IN WATER (2)

All the available data on the solubility of 1-methylnaphthalene in water are summarized in Table 1 with the exception of those of Schwarz and Wasik which have been rejected as they are much more scattered than those in the paper by Schwarz (ref 5). There are insufficient data to warrant plotting.

At 298K, the only temperature where comparison is possible, the data are in excellent agreement and the average value can be Recommended. At other temperatures only the data of Schwarz (ref 5) are available and must thus be considered as Tentative only.

TABLE	2:	Recommended									Solubility	of
		1-Methy	lnar	htha	lene	(1)	in	Wate	c (2	2)		

T/K			Solubility values	
		Reported values ^a 10 ³ g(1)/100g sln		values $(t \sigma_n)^b$ sln $10^6 x_1$
283	2.05*	(ref 5)	2.1	2.7
293	2.56*	(ref 5)	2.6	3.3
			(Table 2 cont	inued next page)

EVALUATOR: COMPONENTS: (1) 1-Methylnaphthalene, C11H10; G.T. Hefter, School of Mathematical [90 - 12 - 0]and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. February 1986. CRITICAL EVALUATION: (continued) Table 2 (continued) T/K Solubility values Reported values a"Best" values $(\pm \sigma_n)^b$ $10^{6}x_{1}$ 10³g(1)/100g sln 10³g(1)/100g sln

 298
 2.58 (ref 2), 2.85 (ref 3)
 2.8 ± 0.2 (R)
 3.5 (R)

 2.95* (ref 5)
 3.35* (ref 5)
 3.4
 4.3

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data. *b* Obtained by averaging where relevant; σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN 1-METHYLNAPHTHALENE (1)

As only the data of Englin *et al*. (ref 1) are available on the solubility of water in 1-methylnaphthalene no Critical Evaluation is possible. However, it may be noted that the solubility values of Englin *et al*. are generally reliable for T < 300K but are larger than Recommended values at higher temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

REFERENCES

- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 3. Mackay, D.; Shui, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.
- 4. Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data 1977, 22, 270-3.
- 5. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 0-50°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	

Solubil	ity of Water in l-Methylnaphthalene.			
<u>t/°C</u>	g(2)/100 g sln	$10^3 x_2$ (compiler)		
0	0.0202	1.59		
10	0.0282	2.22		
20	0.0377	2.97		
30	0.0485	3.82		
40	0.0619	4.87		
50	0.0760	5.97		

AUXILIARY INFORMATION						
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) Not specified.(2) Not specified.					
	ESTIMATED ERROR: Not specified. REFERENCES:					

COMPONENTS :	ORIGINAL MEASUREMENTS:		
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0] (2) Water; H₂O; [7732-18-5]</pre>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski		

The solubility of 1-methylnaphthalene in water at 25°C was reported to be 25.8 mg(1)/kg(2) and 1.81 x 10^{-4} mol(1) L (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 2.58 x 10^{-3} g(1)/100 g sln and 3.27 x 10^{-6} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001	SOURCE AND PURITY OF MATERIALS: (1) source not specified;
mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL was extracted with	analytical grade; used as
hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	(2) doubly distilled; free of trace organics.
	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 1.2 mg(1)/kg(2) (from eight determinations)</pre>
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylnaphthalene; C ₁₁ H ₁₀ ;	Mackay, D.; Shiu, W.Y.
[90-12-0]	J. Chem. Eng. Data 1977, 22,
(2) Water, H of $[7722-10-5]$	399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
one cemperature: 25 c	M.C. haulait-Piison
EXPERIMENTAL VALUES:	
The solubility of 1-methylnaphthalene to be 28.5 mg(1) dm ⁻³ sln and $x_1 = 3$.	
The corresponding mass percent calcul	ated by the compiler
is 0.00285 g(1)/100 g sln.	
e	
AUXILIARI	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
Then the saturated solution was	
decanted and filtered and 50-100 mL extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given	soly. \pm 0.3 mg(1) dm ⁻³ sln
in the paper.	(maximum deviation from several determinations).
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]</pre> (2) Water; H ₂ 0; [7732-18-5]	Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.6-31.7°C	A. Maczynski

Solubility of	1-methylnaphthalene	in water
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t/°C	10 ⁴ mol(1) L ⁻¹	10 ³ g(1)/100 g sln (compiler)	$10^{6}x_{1}$ (compiler)
8.6	1.40 ± 0.03	1.99	2.52
14.0	1.59 ± 0.03	2.26	2.86
17.1	1.61 ± 0.03	2.29	2.90
20.0	1.78 ± 0.02	2.53	3.21
23.0	1.94 ± 0.02	2.76	3.49
25.0	2.11 ± 0.07	3.00	3.80
26.1	2.14 ± 0.02	3.04	3.85
29.2	2.34 ± 0.05	3.33	4.21
31.7	2.55 ± 0.04	3.27	4.59

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Two methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	 (1) source not specified; better than 99.9 mole%, by glc; used as received. (2) distilled over KMnO4 and NaOH and passed through a Sephadex column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above REFERENCES: 	

COMPONENTS: (1) 1-Methylnaphthalene; C ₁₁ H ₁₀ ; [90-12-0] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data <u>1977</u> , 22, 270-3.
VARIABLES:	PREPARED BY:
Temperature: 10-25°C	A. Maczynski

Solubility of 1-methylnaphthalene in water			
t/°C	10 ⁴ mol(1) L ⁻¹	l0 ³ g(l)/l00 g sln (compiler)	10 ⁶ x1 (compiler)
10	1.6	2.3	2.9
14	2.0	2.8	3.6
20	2.0	2.8	3.6
25	2.1	3.0	3.8

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.	 (1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%. (2) distilled from KMnO₄ and passed through a Sephadex column. 	
	ESTIMATED ERROR: temp. \pm 0.1°C soly. \pm 2 x 10 ⁻⁵ mol(1) dm ⁻³	
	REFERENCES :	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylnaphthalene; C ₁₁ H ₁₀ ; [90-12-0]	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES: Temperature: 8.1-28.5°C	PREPARED BY: W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	" Diriu, D. Mackay
EXPERIMENTAL VALUES:	
Solubility of 1-methylnaph	thalene in 0.5 mol(2)/L
<u>t/°C</u>	10 ⁴ mol(1)/L sln
8.1	1.23 1.35
15.5	1.49
17.4	1.53

1.54

1.54

1.63 1.69

1.81

The corresponding mass percent and mole fraction, x_1 , at 25.0°C calculated by the compilers are 2.34 x 10^{-3} g(l)/100 g sln and 3.06 x 10^{-6} .

18.2

20.7

23.3

25.0 28.5

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The solubility of 1-methylnaphthalen in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of 1-methylnaphthalene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent inten- sity was measured at 350 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration was linearly related to the fluores- cence signal. The UV method was used to obtain the absorptivity of 1-methylnaphthalene in ethanol there fore provide an absolute solubility scale for the fluorescence method.	Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 3.6% (author) Temperature ± 0.1°C (author) REFERENCES:	

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COMPONENTS:	EVALUATOR:
<pre>(1) 2-Methylnaphthalene; C₁₁H₁₀; [91-57-6] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for 2-methylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to have been reported on the solubility of water in 2-methylnaphthalene.

TABLE 1: Quantitative Solubility Studies of2-Methylnaphthalene (1) in Water (2)

Reference	Т/К	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in excellent agreement and thus the mean value can be Recommended.

TABLE 2:Recommended (R)Value of the Solubility of2-Methylnaphthalene (1) in Water (2)

т/к	Solubility	y values
	Reported values	"Best" value $(\pm \sigma_n)^a$
	10 ³ g(1)/100g sln	10^{3} g(l)/100g sln $10^{6} x_{1}$
298	2.46 (ref 1), 2.54 (ref 2)	2.50 ± 0.04 (R) 3.2 (R)

a Calculated by averaging; σ_n has no statistical significance.

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61.

2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Methylnaphthalene; C ₁₁ H ₁₀ ; [91-57-6]	Eganhouse, R.P.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

The solubility of 2-methylnaphthalene in water at 25°C was reported to be 24.6 mg(l)/kg(2) and 1.72 x 10^{-4} mol(l) dm⁻³(2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 2.46 x 10^{-3} g(1)/100 g sln and 3.12 x 10^{-6} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	 SOURCE AND FURITY OF MATERIALS: (1) source not specified; analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics.
tors was employed.	ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.5 mg (1)/kg(2) (from eight determinations) REFERENCES:

38_261	321			
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) 2-Methylnaphthalene; C ₁₁ H ₁₀ ;	Mackay, D.; Shiu, W.Y.			
[91-57-6]	J. Chem. Eng. Data <u>1977</u> , 22,			
(2) Water; H ₂ O; [7732-18-5]	399-402.			
2				
VARIABLES:	PREPARED BY:			
One temperature: 25°C	M.C. Haulait-Pirson			
EXPERIMENTAL VALUES:	l			
The solubility of 2-methylnaphthalene	in water at 25°C was reported			
to be 25.4 mg(1) dm ⁻³ sln and $x_1 = 3$.	22×10^{-6} .			
The corresponding mass percent calcul	ated by the compiler			
is 0.00254 g(l)/100 g sln.				
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,			
flask for 24 hrs. and subsequently	commercial highest grade;			
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.			
decanted and filtered and 50-100 mL	(2) doubly distilled.			
extracted with approximately 5 mL of cyclohexane in a separatory				
funnel. After shaking for 2 hrs.				
the cyclohexane extract was removed for analysis. An Aminco-Browman				
spectrophotofluorometer (American				
Instruments Ltd.) was used for analysis. Many details are given	ESTIMATED ERROR:			
in the paper.	soly. \pm 0.2 mg(1) dm ⁻³ sln			

soly. ± 0.2 mg(1) dm⁻³ sln
(maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Ethyl-1,3,5-trimethylbenzene; C ₁₁ H ₁₆ ; [3982-67-0]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	<u> </u>
Solubility of Water in 2-Et	hyl-1,3,5-trimethylbenzene
<u>t/°C</u> <u>g(2)/100 g s</u>	$ln = \frac{10^3 x_2 (compiler)}{10^3 x_2 (compiler)}$
20 0.0259	2.13
30 0.0350 40 0.0461	2.87 3.78
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving	(2) Not specified.
hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) tert-Pentylbenzene; C ₁₁ H ₁₆ ;	Andrews, L.J.; Keefer, R.M.
[2049-95-8]	J. Am. Chem. Soc., <u>1950</u> , 72,
(2) Water; H ₂ O; [7732-18-5]	5034-7.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of tert-pentylbenzene	e in water at 25°C was reported
to be 0.00105 g(1)/100 g sln.	
The corresponding mole fraction, x_1 ,	calculated by the compilers
is 1.27×10^{-6} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated twenty hours in a constant	(1) Eastman Kodak Co. white label; fractionally distilled;
temperature bath at 25°C. A sample	b.p. range 188.0-189.0°C.
(5-20 mL) of the aqueous phase was withdrawn and extracted with a	(2) not specified.
measured volume of hexane (10-50 mL)	(2) not specified.
by shaking in a glass-stoppered	
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was meas-	
ured against a hexane blank on the	
Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) 3-Methylbicyclo[4.4.0]decane	Baker, E.G.			
(2-methyldecalin); C ₁₁ H ₂₀ ;	Am. Chem. Soc., Div. Petrol.			
[2958-76-1]	Chem., Preprints <u>1958</u> , 3, N°4,			
(2) Water; H ₂ O; [7732-18-5]	C61-8.			
VARIABLES:	PREPARED BY:			
One temperature: 25°C	M.C. Haulait-Pirson			
EXPERIMENTAL VALUES: The solubility of 2-methyl- C^{14} decalin in water at 25°C was reported to be 40.6 x 10 ⁻⁹ g(1)/g(2).				

The corresponding mass percentage and mole fraction, x_1 , calculated by the compiler are 4.06 x 10^{-6} g(1)/100 g sln and 4.82 x 10^{-9} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solu- tion of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dis- solved in (2).	 (1) Nuclear Instrument and Chemical Corporation; used as received. (2) distilled.
	ESTIMATED ERROR:
	soly. 20% (standard deviation from 17 replicate runs).
	REFERENCES:
	 Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints- Symposia <u>1956</u>, 1, N°2, 5.

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10 20 30

ORIGINAL MEASUREMENTS:			
Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.			
PREPARED BY: A. Maczynski and M.C. Haulait-Pirson			
EXPERIMENTAL VALUES: Solubility of Water in Hexylcyclopentane $10^4 x_2$ $t/^{\circ}C$ g(2)/100 g sln (compiler)			

0.0052 0.0084 0.0141 4.45 7.19 12.07

AUXILIARY INFORMATION				
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	 Not specified. Not specified. 			
	ESTIMATED ERROR:			
	Not specified.			
	REFERENCES:			

COMPONENTS :	EVALUATOR:
<pre>(1) Undecane; C₁₁H₂₄; [1120-21-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
	December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the system undecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1:	Quantitati	ve Solu	bility	Studies	of
the Un	decane (1)	- Water	(2) S	ystem	

T/K	Solubility	Method
298,313	(2) in (1)	Karl Fischer
298	(1) in (2)	GLC
298	(l) in (2)	GLC
	298,313 298	298,313 (2) in (1) 298 (1) in (2)

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF UNDECANE (1) IN WATER (2)

The available data for the solubility of undecane in water are listed in Table 2.

TABLE 2: Solubility Values of Undecane (1) in Water (2)

<i>т/</i> к	Solubility values			
	Reported values		est" value (± σ_n)	
	10 ⁷ g(1)/100g sln	10 ⁷ g(1)/100g sln	10 ¹⁰ x1	
298	4.4 (ref 2), 3.6 (ref 3)	4.0 \pm 0.4 ^{α}	4.6 ^{<i>a</i>}	

a Order of magnitude only, see text; obtained by averaging.

Although the agreement between the two studies (ref 2,3) is very good considering the very low solubility involved, both values are very much lower than expected from an extrapolation of *n*-alkane solubilities. This may be due (ref 2) to micelle formation. The available data must therefore be considered as Doubtful. The extrapolated value of 1.4 x 10^{-6} g(1)/100g sln ($x_1 = 1.6 \times 10^{-10}$) may be more realistic.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Undecane; C_{11^H24}; [1120-21-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
	December 1985.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN UNDECANE (1)

As only one publication (ref 1) reports solubility data for water in undecane no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg (ref 1) are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. McAuliffe, C. Science <u>1969</u>, 163, 478-9.
- Krasnoshchekova, P.Y.; Gubergrits, M.Y. Neftekhimiya <u>1973</u>, 13, 885-7.

328	38_267
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wate	·
t/°C mg(2)/	<u> </u>
25 69	• .
40 130	^b 11.3×10^{-4}
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and com- pletely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a	 Phillips Petroleum Co.; research grade; 99.33 mole%; passed repeatedly through a column of silica gel until no absorp- tion occurred in the 220 to 340 nm spectral range. distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C solv. a) 0-6%; b) 0-2% (deviations
Beckman KF3 automatic titrimeter.	soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Undecane; C ₁₁ H ₂₄ ; [1120-21-4]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Science 1969, 163, 478-9.
(2) water, n ₂ 0, [//32-10-5]	<u> </u>
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of undecane in water a	at 25°C was reported to be
0.0044 mg(1)/kg(2).	······
The corresponding mass percent and mo	ble fraction, x_1 , calculated
by the compiler are 4.4 x 10^{-7} g(1)/1	.00 g sln and 5.07 x 10^{-10} .
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
E TROD/AFFARATOS/FROCEDURE.	SOURCE AND TORITY OF MATERIALS.
(1) was equilibrated with (2). Glass	(1) not specified.
vials were filled with the saturated aqueous phase. Half of water was	(2) distilled.
then displaced and replaced by air. The vials were then sealed and shaken	
for 2 minutes. The gas phase was	
then displaced through the sample loop of a gas chromatograph for	
analyzing for hydrocarbon content.	
	ESTIMATED ERROR:
	soly. ± 0.0018 mg(1)/kg(2)
	REFERENCES:

330	38_269
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Undecane; C₁₁H₂₄; [1120-21-4] (2) Water; H₂O; [7732-18-5]</pre>	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , <i>13</i> , 885-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	•
The solubility of undecane in water a $x_1 = 4.10 \times 10^{-10}$. The corresponding mass percent calcul 3.6 x 10^{-7} g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor- ously stirred magnetically for 10- 12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP reagent; purity not specified. (2) distilled. ESTIMATED ERROR: not specified. REFERENCES:</pre>

COMPONENTS :	
<pre>(1) Undecane; C_{11^H24}; [1120-21-4] (2) Seawater</pre>	ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
	Neftekhimiya <u>1973</u> , 13, 885 - 8.
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of undecane in seawat 1.0 x 10 ⁻⁶ g(1)/100 g sln. and the c $x_1 = 1.2 \times 10^{-9}$.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solu- tion was then transferred to a closed flask with head space volume equal to solution volume. Hydro- carbon concentration in the head space was determined by gas chroma- tography and the corresponding solution concentration calculated.	SOURCE AND PURITY OF MATERIALS: (1) "chemically pure" (2) distilled water plus salt mixture. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS :	EVALUATOR:
<pre>(1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for acenaphthene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to have been reported for the solubility of water in acenaphthene.

TABLE 1: Ç	Quantitative	Studies	of the	Solubility
of	Acenaphthene	(1) in	Water	(2)

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Eganhouse and Calder (ref 2)	298	GLC
Mackay and Shiu (ref 3)	298	spectrofluorometric
Banerjee et al. (ref 4)	298	radiotracer
Rossi and Thomas (ref 5)	298	GLC, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

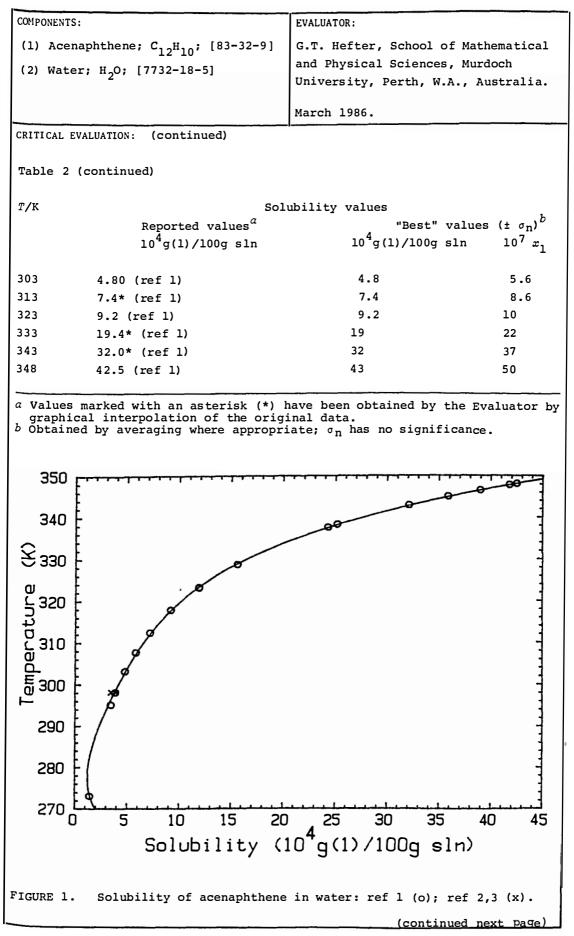
At 298K, the only temperature where comparison is possible (Table 1), the data of Wauchope and Getzen (ref 1), Eganhouse and Calder (ref 2) and Mackay and Shiu (ref 3) are in excellent agreement. The values of Banerjee *et al.* (ref 4) and Rossi and Thomas (ref 5) are respectively very much higher and lower and are therefore rejected.

At other temperatures only the data of Wauchope and Getzen (ref 1) are available and must therefore be regarded as Tentative values.

The solubility values of acenaphthene in water are summarized in Table 2 and plotted in Figure 1.

TABLE	2:	Recommended						Values	for
		Acenar	hth	ene	(1)	in Wate	er (2)		

<i>т/</i> к	Solubili	Solubility values		
	Reported values ^a	"Best" values	(± σ _n) ^b	
	10 ⁴ g(1)/100g sln	10 ⁴ g(l)/100g sln	10 ⁷ x ₁	
273	1.45 (ref 1)	1.5	1.8	
293	3.2* (ref 1)	3.2	3.7	
298	3.88 (ref 1), 3.47 (ref 2), 3.93 (ref 3)	3.8 ± 0.2 (R)	4.4 (<i>R</i>)	
1	• · · · ·	(Table 2 continued n	ext page)	



COMPONENTS: (1) Acenaphthene; C₁₂H₁₀; [83-32-9] (2) Water; H₂O; [7732-18-5] Water; H₂O; [7732-18-5] Warch 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data <u>1972</u>, 17, 38-41.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u>, 14, 1227-9.

5. Rossi, S.S.; Thomas, W.H. Environ. Sci. Technol. <u>1981</u>, 15, 715-6.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

∕°c	mg(l)/kg(2) smoothed with	10 ⁴ g(l)/100 g sln	$10^{7}x_{1}$
_	experiment	(std dev)	(compiler)	(compiler
.0		1.45(0.04)	1.45	1.69
.0	3.57	3.46	3.46	4.04
• 0		3.88(0.07)	3.88	4.53
• 0	4.76, 4.60, 4.72	4.80	4.80	5.61
• 5	6.00, 5.68, 5.73	5.83	5.83	6.81
• 3	6.8, 7.1, 7.0	7.2	7.2	8.4
.7	9.4, 9.4, 9.3	9.2	9.2	10.7
• 0		11.9(0.1)	11.9	13.9
.1	12.5, 12.4, 12.4	11.9	11.9	13.9
.6	15.8, 16.3, 15.9	15.6	15.6	18.2
• 5	25.9, 27.8	24.3	24.3	28.4
• 2	23.7, 23.4, 22.8	25.2	25.2	29.4
• 8	30.1, 34.3, 33.6	32.1	32.1	37.5
.9	35.2	35.9	35.9	41.9
	39.1, 40.1	39.0	39.0	45.6
•7	40.8, 39.3	41.8	41.8	48.8
.0		42.5(0.7)	42.5	49.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass- ware.	

	30_273	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Eganhouse, R.P.; Calder, J.A.	
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of acenaphthene in water at 25°C was reported to be 3.47 mg(l)/kg(2) and 2.2 x 10^{-5} mol(l) dm ⁻³ (2).		
The corresponding mass percent and mo by the compiler are 3.47 x 10 ⁻⁴ g(1)/		
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	 SOURCE AND PURITY OF MATERIALS; (1) source not specified; analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. 	
	<pre>temp. ± 0.5°C soly. ± 0.06 mg(1)/kg(2) (from eight determinations)</pre>	
	REFERENCES:	

ORIGINAL MEASUREMENTS:		
Mackay, D.; Shiu, W.Y.		
J. Chem. Eng. Data <u>1977</u> , 22, 399-402.		
PREPARED BY:		
M.C. Haulait-Pirson		
The solubility of acenaphthene in water at 25°C was reported to be 3.93 mg(1) dm ⁻³ sln and $x_1 = 4.59 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is 3.93 x 10 ⁻⁴ g(1)/100 g sln.		
INFORMATION		
<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.014 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES:</pre>		

338	38_275	
COMPONENTS: (1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] (2) Water; H ₂ 0; [7732-18-5]	Valvani, S.C.	
VARIABLES:	Environ. Sci. Technol. <u>1980</u> , 14, 1227-9. PREPARED BY:	
One temperature: 25°C	G.T. Hefter	
EXPERIMENTAL VALUES: The solubility of acenaphthene in water was reported to be 4.78 x 10^{-5} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction (x_1) solubilities, calculated by the compiler, are 7.37 x 10^{-4} g(1)/100 g sln and 8.60 x 10^{-7} respectively.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: Experiments were performed in sealed stainless steel centrifuge tubes. An excess of acenaphthene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with con- stant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analy- sis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	(2) Distilled.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Rossi, S.S.; Thomas, W.H.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter

The solubility of acenaphthene in distilled water at 25°C was reported to be 2.42 μ g/g, corresponding to a mole fraction, x_1 , of 1.6 x 10⁻⁸. The corresponding mass per cent calculated by the compiler is 2.42 x 10⁻⁴ g(1)/100 g sln.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: Flasks containing 500 mL of water and (1) were placed in a constant tempera-		
ture (±0.1°C) gyrotary shaker (200 Fpm) for at least 24 h. Following a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a separatory funnel. Acenaphthene was isolated from solution by tripli- Cate extraction with 10 mL of hexane, which recovered over 99% of hydro- Carbon as determined in experiments with spiked solutions. Acenaphthene levels in concentrated extracts were determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally deter- mined by ultraviolet spectrophoto- metry. Agreement was typically within 2%. Further details are given in the paper.	(2) Doubly distilled in all-glass apparatus; free of trace organics.	
	ESTIMATED ERROR: Temperature: ±0.1°C	
	Solubility: ±0.02 µg/g (std. dev. for 6 determinations)	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9]	Rossi, S.S.; Thomas, W.H.
(2) Seawater; natural	Environ. Sci. Technol. <u>1981</u> , 15, 715-6.
VARIABLES:	PREPARED BY:
Temperature: 15-25°C	W.Y. Shiu and D. Mackay
Salinity: 35 g/kg sln EXPERIMENTAL VALUES:	
Solubility of Acenar	ohthene in Seawater
10	⁵ Mass ^a
$\frac{t/^{\circ}C}{\mu g(1)/g(2)} g(1)$	$1)/100 \text{ g sln}$ $10^8 \text{ m}_1^{\text{a}}$
15 0.214 20 0.55	2.14 2.56 5.5 6.6
25 1.84	18.4 22.0
a	
^a Calculated by compilers	
AUXILIARY	INFORMATION
 METHOD/APPARATUS/PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Saturated solution was prepared by equilibrating seawater with an ex- cess of hydrocarbon for 24 hrs in a constant temperature gyrotary shaker	Acenaphthene: from Aldrich Chemical Co. of 99% purity and doubly distilled from distilled methanol,
followed by 12 hr stationary period. A 100 mL-aliquot was extracted three	n-Hexane: doubly distilled in glass,
times with n-hexane. The concen- trated hexane extract was analyzed	Seawater: collected off Scripps Pier and was filtered twice
by a gas chromatograph equipped with a flame ionization detector to	through 0.22 pm membrane and twice extracted with
determine the hydrocarbon concentra-	n-hexane then its salinity adjusted to 35 $\%$.
tion.	ESTIMATED ERROR:
	Temp. ±0.1°K
	Soly. ±2%
	REFERENCES :
	· · · · · · · · · · · · · · · · · · ·

38_278

COMPONENTS: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	EVALUATOR: G.T. Hefter, School of Mathematical
(2) Water; H ₂ O; [7732-18-5]	and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	June 1986.

Quantitative solubility data for biphenyl (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in biphenyl.

TABLE 1: Quantitative Solubility Studies of Biphenyl (1) in Water (2)

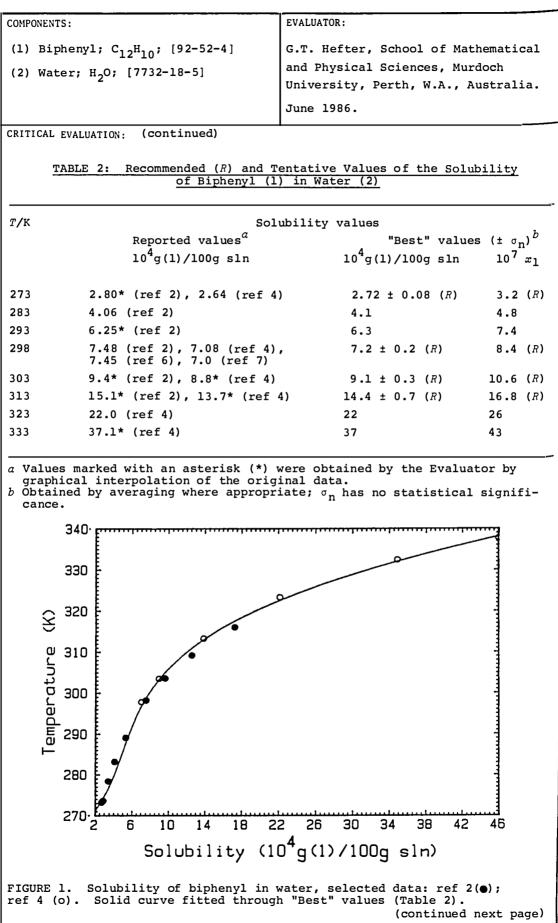
Reference	T/K	Method
Andrews and Keefer (ref 1)	298	spectrophotometric
Bohon and Claussen (ref 2)	274-316	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Ben-Naim et al. (ref 5)	283-323 ^a	spectrophotometric
Eganhouse and Calder (ref 6)	298	GLC
Mackay and Shiu (ref 7)	298	spectrofluorometric
Banerjee et al. (ref 8)	298	HPLC

a Solubility on D₂O also reported.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition Bröllos *et al.* (ref 3) have studied the liquid-liquid phase equilibria in the biphenyl-water system at high temperatures and pressures, and Ben-Naim *et al.* (ref 5) have reported free energies of solution of biphenyl in D_2O .

All the available data on the solubility of biphenyl in water are summarized in Table 2 with the exception of the 298K data of Andrews and Keefer (ref 1) and Banerjee *et al.* (ref 8) which are substantially $(>3\sigma_n)$ lower than all other values at this temperature (ref 2,4,6,7) and are therefore rejected. The data of Ben-Naim *et al.* (ref 5) expressed as free energies of solution have also been excluded.

In general the remaining data are in excellent agreement enabling values to be Recommended over a wide range of temperature. The data from Table 2 are also plotted in Figure 1.



COMPONENTS :	EVALUATOR:
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	June 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

- 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. <u>1949</u>, 71, 3644-7.
- 2. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. <u>1951</u>, 73, 1571-8.
- 3. Bröllos, K.; Peter, K.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. 1970, 74, 682-6.
- 4. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data 1972, 17, 38-41.
- 5. Ben-Naim, A.; Wilf, J.; Yaacobi, M. J. Phys. Chem. 1973, 77, 95-102.
- 6. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 7. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.
- Banerjee, S.; Yalkowski, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u>, 14, 1227-9.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644 - 77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of biphenyl in water a 0.000594 g(l)/100 g sln.	at 25°C was reported to be
The corresponding mole fraction x_1 , calculated by the compilers is 6.9 x 10^{-7} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted	 (1) Eastman Kodak Co. best grade; m.p. 70.0-70.5°C; used as received. (2) pat specified
with a measured volume of hexane (10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank	(2) not specified.
on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Bohon, R.L.; Claussen, W.F.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1951</u> , 73, 1571-8
VARIABLES:	PREPARED BY:
Temperature: 0.4-42.8°C	G.T. Hefter
EXPERIMENTAL VALUES:	
	iphenyl in water
	/100g sln ^a $10^{7}x_{1}$ piler) (compiler)
	.83 3.30
	.97 3.47 .38 3.94
	.64 4.25
	.06 4.74
12.6 4	.58 5.35
	.11 5.96
	.27, 6.15, .48 ^b 8.73 ^b
	.48 8.73 .78 9.08
	.64 11.2
30.4 9	.58 11.2
33.3 11	
34.9 11	
36.0 12 42.8 17	
Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv	rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical
measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assuming	rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.
Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumi b Given in the paper as 7.48 x 10 ⁻³ g(1	rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln.
b Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumi. b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY	rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln.
Measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumi. ^b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY METHOD/APPARATUS/PROCEDURE:	rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS:
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Measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumine ^b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY METHOD/APPARATUS/PROCEDURE: A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe	<pre>rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Matheson Co., purified by recrystallization from absolute methanol. (2) Air-free conductivity water, no further details given</pre>
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Measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumine ^b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY METHOD/APPARATUS/PROCEDURE: A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a guartz cuvette and measured in a Beckman DU spectrophotometer.	<pre>rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Matheson Co., purified by recrystallization from absolute methanol. (2) Air-free conductivity water, no further details given. ESTIMATED ERROR:</pre>
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Measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumi. ^b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY METHOD/APPARATUS/PROCEDURE: A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a Suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a guartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for	<pre>rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Matheson Co., purified by recrystallization from absolute methanol. (2) Air-free conductivity water, no further details given. ESTIMATED ERROR: Temp. ± 0.02°C</pre>
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Measurements. Solubilities were call Beer-Lambert law, the stated cell pa "extinction coefficients" (absorptiv densities. This gave a solubility o converted to g(1)/100g sln by assumin ^b Given in the paper as 7.48 x 10 ⁻³ g(1 AUXILIARY METHOD/APPARATUS/PROCEDURE: A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a Suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls	<pre>rted as "optical density" (absorbance culated by the compiler using the th-length (1 cm) and the authors' ities) and corrected optical f g(1)/L sln which was then ng a solution density of 1.00 kg/L.)/L sln. INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Matheson Co., purified by recrystallization from absolute methanol. (2) Air-free conductivity water, no further details given. ESTIMATED ERROR: Temp. ± 0.02°C Soly. ± 0.5% relative</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-64.5°C	A. Maczynski

Solubility of biphenyl in water

	mg(1)/kg(٨	7
t/°C		smoothed with	10 ⁴ g(1)/100 g sln	$10^{7}x_{1}$
	experiment	(std dev)	(compiler)	(compiler)
			a <i>c i</i>	2 . 0.0
0.0		2.64(0.07)	2.64	3.08
24.6	7.13, 7.29, 7.35	6.96	6.96	8.13
25.0		7.08(0.09)	7.08	8.27
29.9	8.77, 8.64, 8.95	8.73	8.73	10.2
30.3	8.55, 8.54, 8.48	8.88	8.88	10.4
38.4	13.2, 13.3, 13.5	12.7	12.7	14.8
40.1	13.1, 13.4, 13.4	13.8	13.8	16.1
47.5	18.8, 19.0, 18.7	19.5	19.5	22.8
50.0		22.0(0.2)	22.0	25.7
50.1	20.6, 21.6, 21.8	22.1	22.1	25.8
50.2	20.7, 21.8	22.2	22.2	29.9
54.7	28.3, 28.8, 28.8	27.7	27.7	32.4
59.2	36.4, 36.3, 36.0	34.8	34.8	40.7
60.5	40.4	37.2	37.2	43.5
64.5	43.7, 44.7, 46.6	45.9	45.9	53.6

AUXTLTARY	INFORMATION
VOVIDIUVI	THEOREMITON

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated	 Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified. distilled and deionized.
complete extraction. Standard solutions were prepared	ESTIMATED ERROR:
either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass-	<pre>temp. ± 0.5°C soly. see experimental values</pre>
ware.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Ben-Naim, A.; Wilf, J.; Yaacobi, M.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1973</u> , 77, 95-102.
VARIABLES:	PREPARED BY:
Temperature: 10-50°C (282-323 K)	G.T. Hefter

The solubility of biphenyl in water is expressed in terms of the standard free energy of solution, $\Delta \mu_s^0$, determined as:

$$\Delta \mu_{s}^{o} = \lim_{\substack{\rho \neq o \\ \rho \neq o}} \left[-RT \ln(\rho_{s}^{\ell} / \rho_{s}^{g}) \right]$$

where $(\rho_s^{\ell}/\rho_s^{g})_{eq}$ is the Ostwald absorption coefficient and ρ_s^{ℓ} and ρ_s^{g} are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, ${}^{\Delta\mu}{}_{S}$ was fitted to a second degree polynomial of the form:

 $\Delta \mu_{c}^{0} = -14740.4 + 52.057 t - 0.04126 t^{2}$

where t is in °C (10 < t < 50°C) and $\Delta \mu_s^0$ is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were determined spectro- scopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for ca. 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at λ_{max} with a Model 450 Perkin-Elmer spectro- photometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three compartment cell, details of which are given in the paper.	 Fluka; puriss, 99.94%, used as received. Distilled water, further distilled from alk. KMnO₄ and acid K₂Cr₂O₇; κ, 0.8 x 10⁻⁶S cm⁻¹.
	ESTIMATED ERROR: Temperature: $\pm 0.05^{\circ}$ C Solubility: std. dev. in $\Delta \mu^{\circ}$, 22.794 cal/mol.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Eganhouse, R.P.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of biphonul in water a to be 3.47 mg(l)/kg(2) d 4.8 x 10^{-5}	mol(1) dm ⁻³ (2).
The corresponding mass percent and mo	ple fraction, x_1 , calculated
by the compiler are 7.45 x 10^{-4} g(l)/	100 g sln and 8.70 x 10 '.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	 source not specified; analytical grade; used as received; no impurities by glc. doubly distilled; free of trace organics.
	ESTIMATED ERROR:
	<pre>temp. ± 0.5°C soly. ± 0.06 mg(l)/kg(2) (from eight determinations)</pre>
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of biphenyl in water to be 7.0 mg(1) dm ⁻³ sln and $x_1 = 8$.	
The corresponding mass percent calcuing for $(1)^{-4}$ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL	 (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. ± 0.06 mg(1) dm ⁻³ sln (maximum deviation from several determinations.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Water; H ₂ O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. Environ. Sci. Technol. <u>1980</u> , 14, 1227-9.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	G.T. Hefter	

The solubility of biphenyl in water was reported to be 3.91×10^{-5} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1 , solubilities, calculated by the compiler, are 6.03×10^{-4} g(1)/100 g sln and 7.05 x 10^{-7} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Experiments were performed in sealed stainless steel centrifuge tubes. An excess of biphenyl was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at $25 \pm 0.2^{\circ}$ C with con- stant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to $25 \pm$ 0.3° C, following which aliquots of the solution were removed for analy- sis by high-performance liquid chromatography using a Waters M6000A instrument fitted with a μ Cl8 Bondapak column. The mobile phase was a mixture of methanol/water or acenotrile/water. The entire proce- dure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	 (1) Aldrich; purity not specified. (2) Distilled. ESTIMATED ERROR: Temperature: ±0.2°C 	
	Solubility: ±6.0% rel. (represent- ing one std. dev.)	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Biphenyl; C₁₂H₁₀; [92-52-4] (2) Deuterium oxide (Heavy water); D₂O; [7789-20-0]</pre>	Ben-Naim, A.; Wilf, J.; Yaacobi, M. J. Phys. Chem. <u>1973</u> , 77, 95-102.	
VARIABLES:	PREPARED BY:	
Temperature: 10-50°C	G.T. Hefter	

The solubility of biphenyl in heavy water is expressed in terms of the standard free energy of solution, $\Delta \mu_s^0$, determined as:

$$\Delta \mu_{s}^{o} = \lim_{\rho_{q}^{\rightarrow} o} [-RT \ln(\rho_{s}^{\ell}/\rho_{s}^{g})_{eq}]$$

where $(\rho_s^{\ell}/\rho_s^{g})_{eq}$ is the Ostwald absorption coefficient and ρ_s^{ℓ} and ρ_s^{g} are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, $\Delta \mu_{S}^{o}$ was fitted to a second degree polynomial of the form:

 $\Delta \mu_{g}^{0} = -12827.6 + 39.059 t - 0.01945 t^{2}$

where t is in °C (10 < t < 50°C) and $\Delta \mu_{S}^{0}$ is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

 olubilities were determined spectro- copically. Saturated solutions were repared in two ways: (a) direct ixing of benzene and water for ca. 8 h, (b) dissolution of benzene hrough the vapor phase. Absorbances f the solutions and their vapors ere measured directly at λmax with a odel 450 Perkin-Elmer spectrophoto- eter with a thermostatted cell older. Establishment of equilibrium as checked by use of a special three ompartment cell, details of which re given in the paper. (1) Fluka, puriss, 99.94%, used received. (2) Fluka, 99.75%, used as recei (2) Fluka, 99.75%, used as recei
partment cell, details of which ESTIMATED ERROR:
given in the paper.
Temperature: ±0.05°C
Solubility: std. dev. in Δμ ⁰ _S , 270.15 cal/mol.
REFERENCES :

COMPONENTS:	EVALUATOR:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982
CRITICAL EVALUATION:	

The solubility of biphenyl (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 ⁴ g(1)/100 g sln
Paul (ref l)	uv spectral	13-64	6.08 - 3.45
Eganhouse and Calder (ref 2)	GLC	35	4.76

The reported data are all from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the recommended value for the solubility of biphenyl in pure water, the data of Paul and of Eganhouse and Calder are adopted as tentative.

	SOLUBILITY OF	BIPHENYL (1) IN TENTATIVE VALUE	SEAWATER	(2)
<u>т/к</u>		g salts/kg sln		10 ⁴ g(1)/100 g sln
298		35		4.76

REFERENCES

- 1. Paul, M.A. J. Amer. Chem. Soc. 1952, 74, 5274-7.
- 2. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61.

38 288

MPONENTS:	ORIGINAL ME	ASUREMENTS:	
 Biphenyl; C₁₂H₁₀; [92-52-4] Sodium chloride; NaCl; [7732-14-5] Water; H₂O; [7647-18-5] 	Paul, M. J. Am. C 5274-7	hem. Soc. <u>1952</u>	<u>,</u> 74,
2		-	
ARIABLES: Dne temperature: 25°C	PREPARED BY	<i>(</i> :	
Salinity: 13-64 g(3)/kg sln	M. Klein	schmidt and W.	. Shiu
XPERIMENTAL VALUES:			
Solubility of Biphenyl an	d Aqueous	Sodium Chlori	de
mol(2)/L g(2)/kg sln [*] 10 ⁵ m	ol(1)/L	10 ⁴ Mass % [*]	$\frac{10^7 x_1^*}{x_1}$
0.458 26.24 3. 0.687 39.05 3. 0.818 46.28 2. 0.916 51.62 2. 1.145 63.97 2.	98 61 08 79 78 40 34	6.08 5.46 4.62 4.16 4.13 3.54 3.45	7.16 6.49 5.55 5.02 5.01 4.32 4.21
*Calculated by compilers using dens NaCl solutions from ref 1.	ity and o	ther physical	data for
*Calculated by compilers using dens	ity and o	ther physical	data for
*Calculated by compilers using dens NaCl solutions from ref 1.			data for
*Calculated by compilers using dens NaCl solutions from ref 1.	INFORMATION		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4]	Eganhouse, R.P.; Calder, J.A.
(2) Artificial seawater (ref l)	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25.0°C	
Salinity: 35 g/kg sln	M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES:	
	•
The solubility of biphenyl in seawat	ter is reported to be 4.76 mg/kg.
The corresponding mass percent and m	nole fraction, x_1 , calculated
by the compilers are 4.76 x 10^{-4} g(1)	L)/100 g sln and 5.70 x 10^{-7} .
Graphical results for other salinit	les are also reported.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium flask: 1-dm ³ Erlen- meyer flask with ground glass	 analytical grade salts for artificial seawater solution,
stopper and sidearm tap at base	reagent grade.
plugged with glass wool. The mixtures were agitated 12+ hr at	water: doubly distilled
215 rpm on a New Brunswick gyrotary shaker; a 24 hr station-	-
ary equilibrium period followed.	
Hydrocarbons were extracted with doubly-distilled hexane 3 times;	
concentrated by evaporation, with	
losses checked against an internal standard.	ESTIMATED ERROR:
Analysis: gas chromatography	temperature: ± 0.5°C
	<pre>soly: ± 0.293 (95% confidence interval).</pre>
	REFERENCES:
	l. Lyman, J.; Fleming, R.H.;
	J. Mar. Res. <u>1940</u> , 3, 135.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 1,3-Dimethylnaphthalene; C₁₂H₁₂; 	Mackay, D.; Shiu, W.Y.		
[575-41-7]	J. Chem. Eng. Data <u>1977</u> , 22,		
(2) Water; H ₂ O; [7732-18-5]	399-402.		
2			
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of 1,3-dimethylnaphthalene in water at 25°C was reported to be 8.0 mg(1) dm ⁻³ sln and $x_1 = 9.2 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is 8.0 x 10 ⁻⁴ g(1)/100 g sln.			
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.5 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES:</pre>		

	50_231
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1,4-Dimethylnaphthalene; C ₁₂ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[571-58-4]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
2	
VARIABLES:	PREPARED BY:
	T ALLARED DI.
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,4-dimethylnaphth to be 11.4 mg(1) dm ⁻³ sln and $x_1 = 1$	
The corresponding mass percent calcu is 0.00114 g(1)/100 g sln.	lated by the compiler
15 0.00114 g(1)/100 g sin.	
	INFORMATION
	·····
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2)	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. \pm 0.1 mg(1) dm ⁻³ sln
	(maximum deviation from several determinations).
}	REFERENCES :
	,

COMPONENTS:	EVALUATOR:			
<pre>(1) 1,5-Dimethylnaphthalene; C₁₂H₁₂; [571-61-9]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland.			
	June 1986.			
CRITICAL EVALUATION:				
Quantitative solubility data for 1,5-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,5-dimethylnaphthalene.				
TABLE 1: Quantitativ1,5-Dimethylnaphthal	e Solubility Studies of ene (1) in Water (2)			
Reference	T/K Method			
Eganhouse and Calder (ref 1)	298 GLC			
Mackay and Shiu (ref 2)	298 spectrofluorometric			
(Table 2). TABLE 2: Tentative V	an be considered as a Tentative value alue of the Solubility of alene (1) in Water (2)			
T/K Sol	ubility values			
Reported values 10 ⁴ g(1)/100g sln	"Best" value $(\pm \sigma_n)^a$ 10 ⁴ g(1)/100g sln 10 ⁷ x ₁			
298 2.74 (ref 1), 3.38 (ref 2)	3.1 ± 0.3 3.6			
a Obtained by averaging; σ_n has no statistical significance.				
REFERENCES				
<pre>1. Eganhouse, R.P.; Calder, J.A. G 555-61.</pre>	eochim. Cosmochim. Acta <u>1976</u> , 40,			
2. Mackay, D.; Shiu, W.Y. J. Chem.	Eng. Data <u>1977</u> , 22, 399-402.			

COMPONENTS :	ORIGINAL MEASUREMENTS:
 (1) 1,5-Dimethylnaphthalene; C₁₂H₁₂; [571-61-9] (2) Water; H₂O; [7732-18-5] 	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1,5-dimethylnaphth, reported to be 2.74 mg(l)/kg(2) and 2 The corresponding mass percent and mo by the compiler are 2.74 x 10^{-4} g(l),	1.8 x 10^{-5} mol(1) dm ⁻³ (2). ole fraction, x_1 , calculated
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	glc.

COMPONENTS :	ORIGINAL MEASUREMENTS:
 1,5-Dimethylnaphthalene; 	Mackay, D.; Shiu, W.Y.
C ₁₂ H ₁₂ ; [571-61-9]	J. Chem. Eng. Data <u>1977</u> , 22,
	399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1,5-dimethylnaphth to be 3.38 mg(1) dm ⁻³ sln and $x_1 = 3$ The corresponding mass percent calcu	$.77 \times 10^{-7}$.
is $3.38 \times 10^{-4} g(1)/100 g sln.$	
_	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	 (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed	(2) doubly distilled.
for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. ± 0.04 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:

COMPONENTS:	EVALUATOR:
 (1) 2,3-Dimethylnaphthalene; C₁₂H₁₂; [581-40-8] (2) Water; H₂O; [7732-18-5] 	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	June 1986.

Quantitative solubility data for 2,3-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2,3-dimethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of2,3-Dimethylnaphthalene (1) in Water (2)

Reference	Т/К	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of2,3-Dimethylnaphthalene(1) in Water

Т/К	Solubili Reported values	ty values "Best" value (± σ	n) ^a
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln 10	
298	1.99 (ref 1), 3.0 (ref 2)	2.5 ± 0.5 2	.9
a Obtained	l by averaging; σ _n has no statist	ical significance.	
REFERENCES	3		
1. Eganh 555-6	nouse, R.P.; Calder, J.A. <i>Geochi</i>	n. Cosmochim. Acta <u>1976</u> , 4	Ο,

2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

3	8	2	9	6	

56_230	301		
COMPONENTS :	ORIGINAL MEASUREMENTS:		
 (1) 2,3-Dimethylnaphthalene; C₁₂H₁₂; [581-40-8] (2) Water; H₂O; [7732-18-5] 	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski		
EXPERIMENTAL VALUES:			
The solubility of 2,3-dimethylnaphthalene in water at 25°C was reported to be 1.99 mg(l)/kg(2) and 1.3 x 10^{-5} mol(l) dm ⁻³ (2).			
The corresponding mass percent and mo by the compiler are 1.99 x 10 ⁻⁴ g(1)/			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(1) source not specified; analytical grade; used as</pre>		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylnaphthalene; C ₁₂ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[581-40-8]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
<u> </u>	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	·
The solubility of 2,3-dimethylnaphtheter be 2.0 mg(1) dm^{-3} slp and $m = 2$	
to be 3.0 mg(1) dm^{-3} sln and $x_1 = 3.4$	4/ X IU .
The corresponding mass percent calcu	lated by the compiler
is $3.0 \times 10^{-4} g(1)/100 g sln.$	i i i i i i i i i i i i i i i i i i i
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2)	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently	Kodak, or K and K Laboratories, commercial highest grade;
settled at 25°C for at least 48 hrs.	used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	$soly. \pm 0.01 mg(1) dm^{-3} sln$
	(maximum deviation from several determinations).
	REFERENCES:

COMPONENTS:	EVALUATOR: G.T. Hefter, School of Mathematical
<pre>(1) 2,6-Dimethylnaphthalene; C₁₂H₁₂; [581-42-0]</pre>	and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical
(2) Water; H ₂ O; [7732-18-5]	Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	June 1986.

Quantitative solubility data for 2,6-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2,6-dimethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of2,6-Dimethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of 2,6-Dimethylnaphthalene (1) in Water (2)

<i>т</i> /к	Solubility values		
	Reported values 10 ⁴ g(1)/100g sln	"Best" value (± 0 10 ⁴ g(1)/100g sln 10	
298	1.30 (ref 1), 2.0 (ref 2)	1.7 ± 0.4	2.0

a Obtained by averaging; $\sigma_{\texttt{n}}$ has no statistical significance.

REFERENCES

- 1. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61.
- 2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2,6-Dimethylnaphthalene; C ₁₂ H ₁₂ ;	Eganhouse, R.P.; Calder, J.A.	
[581-42-0]	Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski	
EXPERIMENTAL VALUES:		
ENERTHENINE VALUES.		
The solubility of 2,6-dimethylnaphtha		
reported to be 1.30 $mg(1)/kg(2)$ and 8	$3 \times 10^{\circ} \text{ mol}(1) \text{ dm}^{\circ}(2).$	
The corresponding mass percent and mo	ble fraction, x_{1} , calculated	
by the compiler are 1.30 x 10^{-4} g(1),	1 100 g sln and 1.50 x 10 ⁻⁷ .	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE;	SOURCE AND PURITY OF MATERIALS:	
A mixture of 500 mL (2) and 0.001	1	
mol (1) was equilibrated in an	<pre>(1) source not specified; analytical grade; used as</pre>	
Erlenmeyer flask for 12 h (agitation)	analytical grade; used as received; no impurities by	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with	analytical grade; used as received; no impurities by glc.	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc.	analytical grade; used as received; no impurities by	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating	<pre>analytical grade; used as received; no impurities by glc.</pre> (2) doubly distilled; free of	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics.</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc.</pre> (2) doubly distilled; free of	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.04 mg(l)/kg(2) (from eight determinations)</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.04 mg(1)/kg(2)</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.04 mg(l)/kg(2) (from eight determinations)</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.04 mg(l)/kg(2) (from eight determinations)</pre>	
Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec-	<pre>analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics. ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.04 mg(l)/kg(2) (from eight determinations)</pre>	

38_300

38_300	505
COMPONENTS:	ORIGINAL MEASUREMENTS:
 2,6-Dimethylnaphthalene; 	Mackay, D.; Shiu, W.Y.
C ₁₂ H ₁₂ ; [581-42-0]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2,6-dimethylnaphthat to be 2.0 mg(l) dm ⁻³ sln and $x_1 = 2.3$	
The corresponding mass percent calcul is 2.0 x 10^{-4} g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory	(2) doubly distilled.
funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. ± 0.02 mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :
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COMPONENTS:	EVALUATOR:
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂; [1127-76-0]</pre> (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	April 1986.

Quantitative solubility data for 1-ethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1-ethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of1-Ethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Mackay and Shiu (ref 1)	298	spectrofluorometric
Schwarz and Wasik (ref 2)	282-305	spectrophotometric
Schwarz (ref 3)	284-298	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

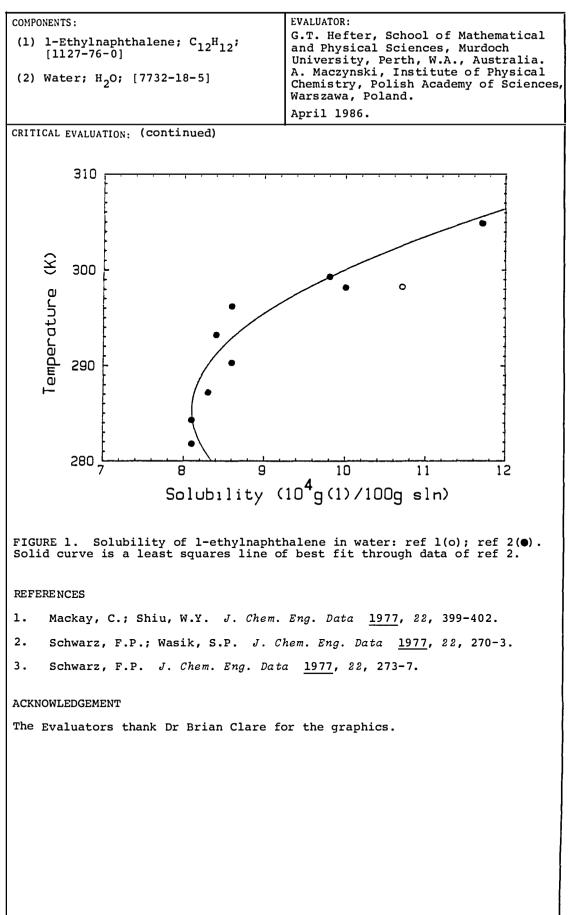
The data available (Table 1) are summarized in Table 2 and plotted in Figure 1. For the purpose of this Evaluation the values of Schwarz (ref 3) are not considered as independent determinations. Nevertheless, the excellent agreement between the data of Schwarz and Wasik (ref 2,3) and Mackay and Shiu (ref 1) at 298K suggests the values of Schwarz and Wasik at other temperatures can be considered as Tentative.

TABLE 2: Recommended (R) and Tentative Solubility Values of1-Ethylnaphthalene (1) in Water (2)

Т/К	Solubility values		
	Reported values ^a	"Best" values	$(\pm \sigma_n)^b$
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁷ <i>x</i> 1
283	8.1 (ref 2), 8.1* (ref 3)	8.1	9.4
293	10.0 (ref 2), 8.5* (ref 3)	8.5	9.8
298	10.7 (ref 1), 10.0 (ref 2), 9.5* (ref 3)	10.1 ± 0.5 (R)	11.6 (<i>R</i>)
303	11.0* (ref 3)	11	13

a Values marked with an asterisk (*) were obtained by the Evaluators by graphical interpolation of the authors' original data.
 b Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)



COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂;</pre>	Mackay, D.; Shiu, W.Y.
[1127-76-0]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	555 402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 1-ethylnaphthalene to be 10.7 mg(1) dm ⁻³ sln and $x_1 = 1$.	
The corresponding mass percent calcul is 0.00107 g(l)/100 g sln.	ated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	 Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed	(2) doubly distilled.
for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. ± 0.3 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:
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20	_303

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 1-Ethylnaphthalene; C₁₂H₁₂; 	Schwarz, F.P.	
[1127-76-0]	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
Temperature: 8.6-31.7°C	A. Maczynski	
EXPERIMENTAL VALUES:		
Solubility of 1-ethylna	phthalene in water	
$t/^{\circ}C$ 10 ⁵ mol(1) L ⁻¹	10^4 g(l)/100 g sln $10^7 x_1$ (compiler) (compiler)	
8.6 5.2 ± 0.3	8.1 9.4	
$\begin{array}{c} 11.1 \\ 5.2 \pm 0.2 \\ 14.0 \\ 5.2 \pm 0.1 \end{array}$	8.1 9.4	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8.3 9.5 8.6 9.9	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8.6 9.9	
$\begin{array}{c} 20.0 \\ 23.0 \\ 5.5 \pm 0.1 \end{array}$	8.6 9.9	
25.0 6.4 ± 0.1	10.0 11.5	
26.1 6.3 ± 0.1	9.8 11.3	
31.7 7.5 ± 0.2	11.7 13.5	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Two methods were used.	(1) source not specified; better	
At 25°C the solubility of (1) in (2)	than 99.9 mole%, by glc; used as received.	
was determined from UV absorption measurements and was used as a	(2) distilled over KMnO ₄ and NaOH	
standard at other temperatures.	and passed through a Sephadex	
At other temperatures the spectrofluorimetry method was used.	column.	
The sealed fluorescence cells		
contained 5 mL of the aqueous		
solution and an excess of (1) were rotated at least 72 h in a water	ESTIMATED ERROR:	
bath, then removed, quickly wiped dry and placed in the fluorimeter.	temp. ± 0.1°C	
	soly. see above	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Ethylnaphthalene; C₁₂H₁₂; [1127-76-0] (2) Water; H₂O; [7732-18-5]</pre>	Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data <u>1977</u> , 22, 270-3.
VARIABLES:	PREPARED BY:
Temperature: 10-25°C	A. Maczynski
EXPERIMENTAL VALUES:	· ·

t/°C 10 ⁵ mol(1) L ⁻¹ 1	0 ⁴ g(l)/l00 g sln (compiler)	$10^{7}x_{1}$ (compiler)
10 5.2 ± 0.2	8.1	9.4
14 5.2 ± 0.1	8.1	9.4
20 6.4 ± 0.1	10.0	11.5
25 6.4 ± 0.1	10.0	11.5

AUXILIARY INFORMATION				
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.	 Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%. distilled from KMnO4 and passed through a Sephadex column. 			
	ESTIMATED ERROR:			
	temp. ± 0.1°C soly. see above			
	REFERENCES:			

ORIGINAL MEASUREMENTS:				
Schwarz, F.P.				
J. Chem. Eng. Data <u>1977</u> , 22, 273-7.				
PREPARED BY:				
W.Y. Shiu, D. Mackay				
W.I. Shiu, D. Mackay				
Solubility of 1-ethylnaphthalene in 0.5 mol(2)/L sln				
10 ⁵ mol(1)/L sln				
3.65				
3.87 4.23				
4.23				
4.38				
4.67				
4.53 4.82				
INFORMATION				
INFORMATION SOURCE AND PURITY OF MATERIALS:				
SOURCE AND PURITY OF MATERIALS:				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ -				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR:				
<pre>SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)</pre>				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author)				
<pre>SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)</pre>				
SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)				
<pre>SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)</pre>				
<pre>SOURCE AND PURITY OF MATERIALS: 1-Ethylnaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author)</pre>				
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38_305

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COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) 2-Ethylnaphthalene; C₁₂H₁₂; [939-27-5]</pre>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40,			
(2) Water; H ₂ O; [7732-18-5]	555-61.			
VARIABLES :	PREPARED BY:			
One temperature: 25°C	A. Maczynski			
EXPERIMENTAL VALUES:				
The solubility of 2-ethylnaphthalene in water at 25°C was reported to be 8.00 mg(l)/kg(2) and 5.1 x 10^{-5} mol(l) dm ⁻³ (2).				
The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 8.00 x 10^{-4} g(1)/100 g sln and 9.22 x 10^{-7} .				
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(1) source not specified; analytical grade; used as received; no impurities by glc.</pre>			
	<pre>(2) doubly distilled; free of trace organics.</pre>			
	ESTIMATED ERROR:			
	<pre>temp. ± 0.5°C soly. ± 0.1 mg(1)/kg(2) (from eight determinations)</pre>			
	REFERENCES:			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) 2-Allyl-1,3,5-trimethylbenzene; C_{12^H16}; [4810-05-3]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.		
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.		
VARIABLES:	PREPARED BY:		
Temperature: 20-40°C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
Solubility of Water in 2-Allyl-1,3,5-trimethylbenzene			
<u>t/°C</u> <u>g(2)/100 g s</u>	$\ln \qquad 10^3 x_2 (compiler)$		
20 0.0246 30 0.0331 40 0.0438	1.15 1.54 2.04		
AUXILIARY	INFORMATION		
L	SOURCE AND PURITY OF MATERIALS:		
Component (1) was introduced into a	(1) Not specified.		
thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) Not specified.		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6. PREPARED BY: A. Maczynski and Z. Maczynska pyl-1,3,5-trimethylbenzene $10^{3} x_{2}$ (compiler) 2.29 3.08 4.09
Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6. PREPARED BY: A. Maczynski and Z. Maczynska pyl-1,3,5-trimethylbenzene $\frac{10^3 x_2 (compiler)}{2.29}$ 3.08
A. Maczynski and Z. Maczynska ppyl-1,3,5-trimethylbenzene $\frac{10^{3} x_{2} \text{ (compiler)}}{2.29}$ 3.08
A. Maczynski and Z. Maczynska ppyl-1,3,5-trimethylbenzene $\frac{10^{3} x_{2} \text{ (compiler)}}{2.29}$ 3.08
pyl-1,3,5-trimethylbenzene <u>10³ x₂ (compiler)</u> 2.29 3.08
<u>10³ x₂ (compiler)</u> 2.29 3.08
<u>10³ x₂ (compiler)</u> 2.29 3.08
2.29 3.08
3.08
INFORMATION
SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR:
Not specified. REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Phenylhexane; C ₁₂ H ₁₈ ; [1077-16-3]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.		
(2) Water; H ₂ O; [7732-18-5]	Vodnye. Resursy. <u>1975</u> , 2, 170-3.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	A. Maczynski		
EXPERIMENTAL VALUES:			
The solubility of 1-phenylhexane in w 0.0021 mg(1) cm ⁻³ sln. The corresponding mass percent and mo by the compiler are 0.00021 g(1)/100 assumption that 1.00 L sln = 1.00 kg	ble fraction, x_1 , calculated g sln and 2.4 x 10^{-7} . The		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The colubility of (1) is (2) use	(1) described is ref (1)		
The solubility of (1) in (2) was determined by glc.	(1) described in ref (1).		
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.	(2) distilled.		
	ESTIMATED ERROR:		
	temp. ± l°C		
	REFERENCES:		
	1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885.		

COMPONENTS:	EVALUATOR:
<pre>(1) Dodecane; C₁₂H₂₆; [112-40-3] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	April 1986.

Quantitative solubility data for the system dodecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Dodecane (1) - Water (2) System

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DODECANE (1) IN WATER (2)

The solubility of dodecane in water has been reported in only two publications, both at 298K (Table 1). The agreement between the two studies is very poor with Franks value (ref 2) considerably higher than that reported by Sutton and Calder (ref 3). Support for the lower value comes from extrapolation of the lower *n*-alkane solubilities. However, there is sufficient uncertainty in this extrapolation to preclude rejection of the higher value at this time. The available data are summarized in Table 2.

TABLE 2: Tentative Solubility Values of Dodecane (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁷ g(1)/100g sln	"Best" value ^a 10 ⁷ g(1)/100g sln	10 ¹⁰ <i>x</i> 1
298	8.42 (ref 2), 3.7 (ref 3)	3.7	3.9

a Datum from ref 3 preferred as Tentative value; see text.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Dodecane; C₁₂H₂₆; [112-40-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	April 1986.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN DODECANE (1)

As only the data of Schatzberg (ref 1) are available no Critical Evaluation is possible. However, it may be noted that the values of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.

2. Franks, F. Nature (London) 1966, 210, 87-8.

3. Sutton, C.; Calder, J.A. Environ. Sci. Technol. 1974, 8, 654-7.

	50_511
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wate	r in dodecane
t/°C mg(2)/k	g sln $\frac{x_2}{2}$
25 65	
40 127	
^a See "Estimated Error"	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and com- pletely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.	 (1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. a) 0-6%; b) 0-2% (deviations from the mean) REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Franks, F.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1966</u> , 210, 87-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of dodecane in water a	t 25°C was reported to be
in mole fraction $x_1 = 8.9 \times 10^{-10}$.	
The corresponding mass percent calcul	ated by the compiler is
$8.42 \times 10^{-7} g(1)/100 g sln.$	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analysis was performed by gas liquid chromatography. After	<pre>(1) Fluka; purum grade; purity > 97% (chromatographic</pre>
equilibrating the $(1)/(2)$ mixtures in a thermostat, up to 0.5 mL of the	analysis).
aqueous phase was injected into the	(2) not specified.
fractionator fitted to the chroma- tographic column, and (2) was	
removed by "Drierite". The (1) concentrations were obtained from	
the peak areas, after initial calibrations.	
	ESTIMATED ERROR:
	soly. ± 12%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3] (2) Water; H ₂ O; [7732-18-5]	Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

```
The solubility of dodecane in water at 25°C was reported to be 3.7 \times 10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 of 4 \times 10^{-10}.
```

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

.

- (1) Analabs Inc., 99+%.
- (2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C soly. ± 16%

REFERENCES:

38 314

COMPONENTS:	EVALUATOR:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

The solubility of dodecane (1) in seawater (2) at 298 K has been reported in three works:

Authors	Method	Salinity g salts/kg sln	10 ⁷ g(l)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	6	5
Sutton and Calder (ref 2)	GLC	35	2.9
Button (ref 3)	isotopic	12	1.74

The reported data are all from different salinities which precludes direct comparison. Since the data are in only fair agreement with each other and with the reported values for the solubility of dodecane in pure water, all three values are adopted as tentative.

	SOLUBILITY O	F DODECANE (1) IN TENTATIVE VALUE	(2)
т/к		g salts/kg sln	g(l)/100 g sln
298		35	2.9×10^{-7}

REFERENCES

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya, <u>1973</u>, 13, 885-8.
- 2. Sutton, C.; Calder, J.A. Environ. Sci. Technol. 1974, 8, 654-7.
- 3. Button, D.K. Geochim. Cosmochim. Acta 1975, 40, 435-40.

00170170470	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.
(2) Seawater	
	Neftekhimiya <u>1973</u> , 13, 885 - 8.
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of dodecane in seawate	ar was reported to be
	-
5×10^{-7} g(1)/100 g sln. and the cor:	responding mole fraction,
$x_1 = 5.0 \times 10^{-10}$.	
1	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution was prepared	(1) "chemically pure"
by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs.	(2) distilled water plus salt
in a flask placed in a temperature	mixture.
controlled bath. A sample of solu- tion was then transferred to a	
closed flask with head space volume	
equal to solution volume. Hydro- carbon concentration in the head	
space was determined by gas chroma-	
tography and the corresponding solution concentration calculated.	ESTIMATED ERROR:
	not specified.
	REFERENCES :

38_316

383
ORIGINAL MEASUREMENTS:
Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
PREPARED BY: P.A. Meyers and D. Shaw
er was reported to be .1 x 10 ⁻¹⁰ .
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre> ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	·
(1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3]	Button, D. K.
(2) Salt mixture (ref 1)	Geochim. Cosmochim. Acta <u>1975</u> , 40, 435-40.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C Constant salinity: 12 g(2)/kg sln Different periods of standing	P. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
gently stirring for 1	in saline medium after week and then remaining he periods shown
<u>Time, Weeks</u>	Dodecane, µg(l)/L(2)
1 8 16	2.16 ± 0.03 1.80 ± 0.02 1.78 ± 0.02
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Dodecane solutions were prepared in a chemically defined solution resem- bling dilute seawater. In addition to the mineral salts and vitamins reported (ref 1), the solution con- tained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121°C for 30 min), $0.8 \ \mu L$ of ¹⁴ C-dodecane was sprayed on to the medium surface to form a thin film. Gentle sub- surface agitation was induced by a 3 in magnet rotating at 60 rev/min	Amersham Searle Corp. (Arlington Heights, Ill.) supplied the [1- ¹⁴ C] dodecane, 27 µCi/µmol. It was ac- companied by a gas chromatogram of the preparation showing a single peak at the appropriate location.
against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples col- lected from a port at the bottom of the carboy. The system was stirred for 1 week and then allowed	ESTIMATED ERROR: Experimental error is estimated at ± 1%.
to stand. Equilibrium appeared to have been achieved within 8 weeks.	REFERENCES: 1. Button, D. K. Limnol. Oceanogr. <u>1969</u> , 14, 95-100.

3	8	3	1	8

COMPONENTS:	EVALUATOR:
<pre>(1) Fluorene; C₁₃H₁₀; [86-73-7] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	April 1986.

Quantitative solubility data for fluorene (1) in water (2) have been reported in the publications listed in Table 1. No solubility data for water in fluorene have been reported.

TABLE 1:		Solubility Studies of
	Fluorene (1)	in Water (2)

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Mackay and Shiu (ref 2)	298	spectrofluorometric
May et al. (ref 3)	298	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The solubility values are also summarized in Table 2 and plotted in Figure 1.

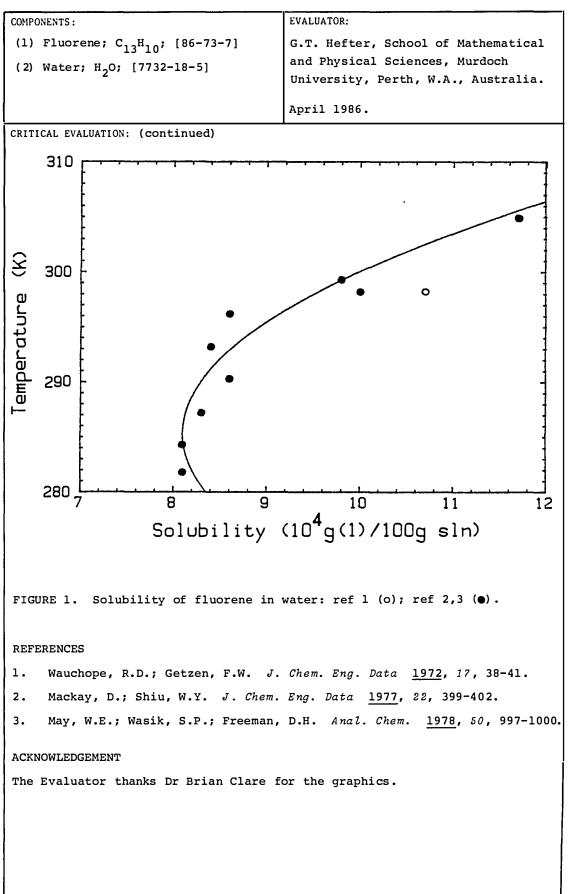
At 298K, the only temperature where comparison is possible, the available data (ref 1-3) are in good agreement and the average value can be Recommended. At other temperatures only the values of Wauchope and Getzen (ref 1) are available and are therefore regarded as tentative.

 TABLE 2:
 Recommended (R) and Tentative Solubility Values of

 Fluorene (1) in Water (2)

<i>т</i> / к	Reported values ^a	ty values	b
		"Best" value	es (± ơ _n)
	10 ⁴ g(1)/100g sln	10 ⁴ g(1)/100g sln	10 ⁶ x ₁
273	0.66 (ref 1)	0.7	0.8
298	1.90 (ref 1), 1.98 (ref 2), 1.685 (ref 3)	1.9 ± 0.1 (R)	2.1 (<i>R</i>)
303	2.4* (ref 1)	2.4	2.6
313	3.8* (ref 1)	3.8	4.1
323	6.29 (ref 1)	6.3	6.8
333	10.4* (ref 1)	10	11
343	18.5* (ref 1)	19	21
a Value	s marked with an asterisk (*) were	obtained by the Evalua	ator by

b Obtained by averaging where appropriate; σ_n has no statistical significance. (continued next page)



COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

EXPERIMENTAL VALUES:

t/°C	mg(l)/kg(experiment	z) smoothed with (std dev)	10 ⁴ g(1)/100 g sln (compiler)	10 ⁷ x1 (compiler)
0.0		0.66(0.01)	0.66	7.2
24.6	1.93, 1.87, 1.88	1.86 1.90(0.03)	1.86 1.90	20.2 20.6
25.0	2 41 2 22 2 24		2.37	20.8
29.9 30.3	2.41, 2.33, 2.34 2.10, 2.25, 2.23		2.37	26.1
30.3	3.72, 3.73		3.53	38.2
	3.88, 3.84, 3.85		3.84	41.6
40.1	5.59, 5.62, 5.68		5.54	60.0
50.0	5.59, 5.02, 5.00	6.29(0.05)	6.29	68.2
50.1	6.31, 6.42, 6.54		6.32	68.5
	6.27	6.35	6.35	68.8
	8.31, 8.41, 8.56		8.02	86.9
	10.5, 10.5	10.2	10.2	110
60.5	10.7, 11.0, 11.6	10.9	10.9	118
65.1		14.1	14.1	153
70.7	18.5, 18.5, 18.9	19.3	19.3	209
71.9	18.8	20.6	20.6	223
73.4	21.5	22.5	22.5	244
75.0		24.7(0.4)	24.7	268
		AUXILIARY INFOR	MATION	

Approximately 20 g of (1) was placed in each of three 250-mL glass-(1) Baker reagent; recrystallized three times from ether; stoppered flasks with (2). The flasks were suspended in an open vacuum-sublimed twice; purity not specified. water bath and shaken gently from one to three weeks between measure-(2) distilled and deionized. ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass-**REFERENCES:** ware.

ESTIMATED ERROR:

temp. ± 0.5°C soly. see experimental values above

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of fluorene in water to be 1.98 mg(1) dm ⁻³ sln and $x_1 = 2$ The corresponding mass percent calculis 1.98 x 10 ⁻⁴ g(1)/100 g sln.	$.14 \times 10^{-7}$.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled.</pre>
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. ± 0.04 mg(1) dm ⁻³ sln (maximum deviation from several determinations.)
	REFERENCES :

38_321	389
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Water; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
£	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of fluorene in water 1.685 mg(1)/kg(2). The corresponding mass percent and m by compiler are 1.685 x 10 ⁻⁴ g(1)/10	ole fraction, x_1 , values calculated
AUXILIARY	INFORMATION
ME THOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The dynamic coupled column liquid chromatography (DCCLC) method was	(1) commercial product; less than 3% impurities.

based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con-centration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromato-graphic process that has been

described in ref 1.

- (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

```
temp. ± 0.05°C
soly. ± 0.005 mg(1)/100 kg(2)
      (standard deviation)
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REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. <u>1975</u>, 13, 535.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Fluorene; C ₁₃ H ₁₀ ; [86-73-7]	May, W.E.; Wasik, S.P.; Freeman, D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997–1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of fluorene in aqueou	is sodium chloride is
reported in terms of the Setschenow	equation:
log(S _o /S) = K _s C _s	
where;	
S _o is the solubility	of (l) in water (mg/L)
S is the solubility of	of (l) in saline solution (mg/L)
K _c is the Setschenow	constant (L/mol)
5	on of sodium chloride (mol/L)
s evaluating the equation for S over t	
$K_{s} = 0.267$ with $S_{o} = 1.685$.	S S
The corresponding mass percent and π	-
_	pilers are $1.20 \times 10^{-4} g(1)/100 g sln$
and 1.30×10^{-7} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide
with a superficially porous bonded	and passed through an XAD-2 column.
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed	
through for extraction. The	
extract was introduced into a liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a UV detector.	temp ± 0.05°C
	REFERENCES :
1	

CONDONIDIMO -	
COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Diphenylmethane; C₁₃H₁₂; [101-81-5]</pre>	Andrews, L.J.; Keefer, R.M.
	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
(2) Water; H ₂ O; [7732-18-5]	5044-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of diphenylmethane in	water at 25°C was reported to be
$1.41 \times 10^{-4} g(1)/100 g sln.$	
The corresponding mole fraction, x_1 , is 1.51 x 10 ⁻⁷ .	value calculated by compiler
is 1.51 x 10 .	
	1
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant	 Eastman Kodak Co., best grade; purified by fractional freezing;
temperature bath at 25°C. A sample	m.p. 25°C.
(5-20 mL) of the aqueous phase was withdrawn and extracted with a mea-	(2) not specified.
sured volume of hexane (10-50 mL) by shaking in a glass-stoppered	
Erlenmeyer flask. Next, the absorb- ance of the hexane phase was mea-	
sured against a hexane blank on the	
Beckman spectrophotometer.	ESTIMATED ERROR:
	not specified.
	Specifica.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1,4,5-Trimethylnaphthalene; 	Mackay, D.; Shiu, W.Y.
C ₁₃ H ₁₄ ; [213-41-1]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	333-402.
_	
VARIABLES :	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	•
The solubility of 1,4,5-trimethylnaph to be 2.1 mg(1) dm ⁻³ sln and $x_1 = 2.1$	thalene in water at 25°C was reported 5×10^{-7}
$\begin{bmatrix} co be 2.1 & mg(1) & m \\ 1 & 2.1 \end{bmatrix}$	
The corresponding mass percent calcul	ated by the compiler
is 2.1 x 10^{-4} g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD /AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL	 Aldrich Chemicals, Eastman Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently	commercial highest grade;
settled at 25°C for at least 48 hrs. Then the saturated solution was	used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. \pm 0.1 mg(1) dm ⁻³ sln (maximum deviation from several
	determinations).
	REFERENCES :

38_3	25
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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) (2-Ethylcyclopentyl) benzene; C_{13^H18}; [4810-07-5]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	
	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in (2-	Ethylcyclopentyl) Benzene
<u>t/°C</u> <u>g(2)/100 g sl</u>	$\frac{10^3 x_2 \text{ (compiler)}}{10^3 x_2 \text{ (compiler)}}$
10 0.0103	1.00
20 0.0168 30 0.0273	1.62 2.64
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a	(1) Not specified.
thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was	(2) Not specified.
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Cyclopentyloctane; C ₁₃ H ₂₆ ; [4810-01-9]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson
Temperature: 10-30 C	A. Maczynski and M.C. Maulait Filson
EXPERIMENTAL VALUES:	
Solubility of Water in	n 2-Cyclopentyloctane
<u>t/°C</u> g(2)/100 g s	$\frac{10^4 x_2}{(\text{compiler})}$
10 0.0048	4.86
20 0.0075 30 0.0122	7.59 12.34
	i i
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hours with (2). Next, calcium	(2) Not specified.
hydride was added and the evolving hydrogen volume measured and hence	
the concentration of (2) in (1) was evaluated.	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	not specified.
	REFERENCES :
1	

COMPONENTS:

(1) Tridecane; C ₁₃ H ₂₈ ; [629-50-5] (2) Water; H ₂ O; [7732-18-5]	Schatzberg, P. J. Phys. Chem. <u>1963</u> , 67, 776-9.	
VARIABLES: Temperature: 25-40°C	PREPARED BY: M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of wate:	r in tridecane	
t/°C mg(2)/1	$\frac{x_2}{2}$	
25 60 [°] 40 123 ¹		
^a See "Estimated Error"		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and com- pletely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.	<pre>(1) Phillips Petroleum Co.; research grade; 99.73 mole %; passed repeatedly through a column of silica gel until no absorp- tion occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. a) 0-6%; b) 0-2% (deviations from the mean) REFERENCES:</pre>	
Hww 2-AA		

ORIGINAL MEASUREMENTS:

COMPONENTS:	EVALUATOR:
<pre>(1) Anthracene; C₁₄H₁₀; [120-12-7] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

Quantitative solubility data for anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in anthracene.

TABLE 1: Quantitative Solubility Studies ofAnthracene (1) in Water (2)				
Reference T/K Method				
Davis <i>et al</i> . (ref l)	300	nephelometric		
Klevens (ref 2)	298	spectrophotometric		
Wauchope and Getzen (ref 3)	273-348	spectrophotometric		
Mackay and Shiu (ref 4) 298 spectrofluorometric				
Schwarz (ref 5)	282-305	spectrophotometric		
May et al. (ref 6)	278-302	chromatographic		

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the 300K datum of Davis *et al.* (ref 1) which is several orders of magnitude lower than all other values, all the available data on the solubility of anthracene in water are summarized in Table 2. Selected data are also plotted in Figure 1.

At 298K the data are clustered around two values (Table 2). A possible explanation for this (ref 6) is that most commercial preparations of anthracene contain about 2% phenanthrene. Although isomeric with anthracene, phenanthrene is about 20 times more soluble which could result in higher observed values for analytical methods such as spectrophotometry which do not distinguish between the two isomers. However, at the present time there are insufficient data to justify rejection of the higher values. Clearly, a careful reinvestigation of this system is justified.

At temperatures lower than 298K the data of Schwarz (ref 5) and May *et al*. (ref 6) are in good agreement. However, in view of the discrepancies at 298K these values are regarded only as Tentative.

At T > 298K only the data of Wauchope and Getzen (ref 3) are available and in view of the disagreement at 298K must also be regarded as very tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
<pre>(1) Anthracene: C₁₄H₁₀; [120-12-7] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	February 1986.

CRITICAL EVALUATION: (continued)

TABLE	2:	Tentative	Value	es of	the	Solu	bility	of
·······		Anthracene	e (1)	in V	later	(2)		

T/K	Solubility Reported values ^a 10 ⁶ g(1)/100g sln	values "Best" values 10 ⁶ g(1)/100g sln	
273	2.2 (ref 3)	2.2	0.22
283	2.38* (ref 5), 1.74* (ref 6)	2.1 ± 0.3	0.21
293	3.48* (ref 5), 3.23* (ref 6)	3.4 ± 0.1	0.34
298	7.5 (ref 2), 7.5 (ref 3) 7.3 (ref 4), 4.46* (ref 5), 4.46 (ref 6)	6.2 ± 1.5 [°]	0.62 [°]
303	8.0* (ref 3)	8 ^{<i>c</i>}	8 <i>°</i>
313	16* (ref 3)	16 ^{<i>c</i>}	16 <i>°</i>
323	28.6 (ref 3)	29 ^{<i>c</i>}	29 <i>°</i>
333	51* (ref 3)	51 <i>°</i>	51 [°]
343	91 (ref 3)	91 [°]	91 [°]

a Values masked by an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data. b Obtained by averaging where appropriate; σ_n has no statistical signifi-

cance. *c* See text however.

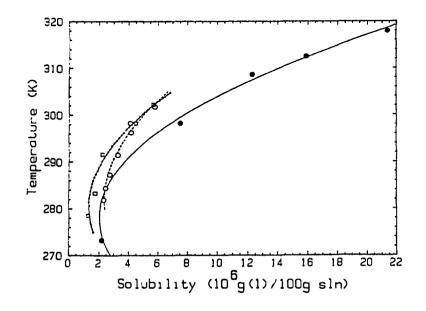


FIGURE 1. Solubility of anthracene in water, selected data: ref 3 (\bullet), solid curve; ref 5 (o), broken curve; ref 6 (\Box), broken curve.

(continued next page)

COMPONENTS :	EVALUATOR:			
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	G.T. Hefter, School of Mathematical			
(2) Water; H ₂ O; [7732-18-5]	and Physical Sciences, Murdoch			
2	University, Perth, W.A., Australia.			
	February 1986.			
CRITICAL EVALUATION: (continued)				
REFERENCES				
 Davis, W.W.; Krahl, M.E.; Cloves 108-10. 	, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64,			
2. Klevens, H.B. J. Phys. Chem. <u>1</u>	<u>950</u> , <i>54</i> , 283-298.			
3. Wauchope, R.D.; Getzen, F.W. J.	Chem. Eng. Data <u>1972</u> , 17, 38-41.			
4. Mackay, D.; Shiu, W.Y. J. Chem.	Eng. Data <u>1977</u> , 22, 399-402.			
5. Schwarz, F.P. J. Chem. Eng. Dat	a <u>1977</u> , 22, 273-7.			
 May, W.E.; Wasik, S.P.; Freeman, 1000. 	D.H. Anal. Chem. <u>1978</u> , 50, 997-			
ACKNOWLEDGEMENT				
The Evaluator thanks Dr Brian Clare f	or the graphics.			

30_329	399
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Water; H ₂ O; [7732-18-5]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	1
Solubility of anth: <u> t/°C</u> 27	racene in water $\frac{10^7 \text{ g(1) L}^{-1} \text{ (2)}}{7.5 \pm 0.8}$
	7.2 ± 0.5 7.5 ± 0.5
The best value recommended by the au Assuming that 1.00 L sln = 1.00 kg mass percent and mole fraction, x_1 , 6 7.5 x 10^{-8} g(1)/100 g sln and 7.6 x 1	sln, the corresponding values of calculated by the compiler are
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) Eastman Kodak Company, 450x; m.p. range 215.6-216.5°C; used as received; (cf. ref 2). (2) dust-free.
	ESTIMATED ERROR: temp. ± 3°C soly. see above.
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101.</pre>

 101.
 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	
	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	·
The solubility of anthracene in water 7.5 x 10^{-5} g(1) dm ⁻³ sln and 4.47 x 1 Assuming that 1.00 dm ³ sln = 1.00 dm ³ and mole fraction, x_1 , calculated by 100 g sln and 8.07 x 10^{-9} .	.0 ⁻⁷ mol(1) dm ⁻³ sln. sln the dorresponding mass percent
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES :

(2) Water; H ₂ O; [7732-18-5]		J. Chem. Er 38-41.	ng. Data <u>1</u>	<u>.972</u> , 17,
VARIABLES:		PREPARED BY:		
Temperature: 0-75°C		A. Maczynsł	ki	
EXPERIMENTAL VALUES:	I			
Solubility of anthracene in water				
mg(1)/kg(2)		1.5	(1) (100	1 1.8
	thed wi td <u>de</u> v)	$\frac{10^{\circ} \text{ g}}{2}$	(1)/100 g s compiler)	$\frac{10^8 x_1}{(\text{compiler})}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	159 214 249 286(0.00 288 372 481 66 66 68 90 95 02	02)	0.22 0.75 1.23 1.59 2.14 2.49 2.86 2.88 3.72 4.81 6.6 6.8 9.0 9.5 10.2 12.1 12.3	0.22 0.76 1.24 1.61 2.16 2.52 2.89 2.91 3.76 4.86 6.7 6.9 9.1 9.6 10.3 12.2 12.4
A	UXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:		
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete		three t vacuum-	imes from sublimed t not specif	wice; ied.
extraction. Standard solutions were prepared		ESTIMATED ERROR:		
either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass- Ware.		temp. ± 0.5 soly. see e above REFERENCES:	experimenta	l values

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

38_331

COMPONENTS:

(1) Anthracene; C₁₄H₁₀; [120-12-7]

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of anthracene in water to be 0.073 mg(l) dm ⁻³ sln and $x_1 = 7$	
The corresponding mass percent calcul is 7.3 x 10^{-6} g(1)/100 g sln.	ated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL	(2) doubly distilled.
extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	
Instruments Ltd.) was used for analysis. Many details are given	ESTIMATED ERROR:
in the paper.	<pre>soly. ± mg(1) dm⁻³ sln (maximum deviation from several determinations.)</pre>
	REFERENCES:
	l <u></u>

3	8	3	3	3

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Schwarz, F.P.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data, <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.6 - 31.3°C	A. Maczynski

EXPERIMENTAL VALUES:	
Solubility of Ant	nracene in Water
	hracene in Water $g(1)/100g sln$ $10^9 x_1$ $(compiler)$ $(compiler)$ 2.33 2.36 2.44 2.47 2.57 2.59 2.74 2.77 2.96 3.00 3.23 3.26 3.96 4.00 4.17 4.21 4.10 4.14 4.76 4.81 5.79 5.85 6.95 7.02
AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
Two methods were used. At 25°C the solubility of (1) in (2) was deter- mined from UV absorption measurements	 (1) Source not specified; better than 99 mole %, by glc, used as received.
and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solu- tion and an excess of (1) were rotated at least 74 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	(2) Distilled over KMnO ₄ and NaOH and passed through ⁴ a Sephadex column.
	ESTIMATED ERROR:
	Temperature: ±0.1°C
	Solubility: See above.
	REFERENCES:
	l

	COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]		May, W.E.; Wasik, S.P.; Freeman, D.H.			
(2) Water; H ₂ O; [7732-18-5]		Anal. Chem. <u>1978</u> , 50, 175-9 and 997-1000.			
VARIABLES:					
VARIABLES:		PREPARED BY:			
Temperature: 5.2-29.0°C		A. Maczynski			
EXPERIMENTAL VALUES:					
Solubi	lity of anth	acene in water			
t/°C μg(l)/	kg(2)	10 ⁶ g(1)/100 g sln (compiler)	$10^{9}x_{1}$ (compiler)		
5.2 12.7 ±	0.4	1.27	1.28		
10.0 17.5 ±		1.75	1.77		
14.1 22.2 ±		2.22	2.24		
18.3 29.1 ±	0.6	2.91	2.94		
22.4 37.2 ±	1.1	3.72	3.76		
24.6 43.4 ±	0.1	4.34	4.39		
25.0 44.6 ±	0.2	4.46	4.51		
28.7 55.7 ±	0.7	5.57	5.63		
29.0 57.0 ±	3.0	5.7	5.76		
, , , , , , , , , , , , , , , , , , ,	001 1 + 0.003	$17 t^2 + 0.0013 t^3$			
rg(1), rg(2)	801 L + 0.005	7 E + 0.0013 E			
		INFORMATION			
METHOD/APPARATUS/PROCEDURE:			ALS;		

38_335

COMPONENTS :	EVALUATOR:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

The solubility of anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 ⁶ g(1)/100 g sln
Schwarz (ref 1)	uv spectral	30	3.55
May et al. (ref 2)	HPLC	35.0	3.11

The reported data are from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the tentative value for the solubility of anthracene in pure water, the data of Schwarz, and May *et al.* are adopted as tentative. Schwarz also reports data over the temperature range 281-303 K.

	SOLUBILITY OF	ANTHRACENE (1) IN	SEAWATER (2)
		TENTATIVE VALUE	
<u>т/к</u>		g salts/kg sln	10 ⁶ g(1)/100 g sln
298		35.0	3.11

REFERENCES

- 1. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

06	38_33
OMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	Schwarz, F.P.
<pre>(2) Sodium chloride NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water: H ₂ O; [7732-18-5]	
ARIABLES:	PREPARED BY:
Temperature: 8.2-30.2°C Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay
XPERIMENTAL VALUES:	
Solubility of Anthrace	ene in 0.5 mol(2)/L
t,°C	10 ⁷ mol(l)/L sln
8.2	0.93
8.6	1.01
11.7	1.22
19.2 21.5	1.47 1.68
21.5	2.04
25.3	1.92
27.1 30.2	2.02 2.46
calculated by the compilers are 3.	1 mole fraction x_1 , at 25.0°C .55 x 10 ⁻⁶ g(1)/100 g sln and
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ .	
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY	.55 x 10 ⁻⁶ g(l)/l00 g sln and INFORMATION
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl	.55 x 10 ⁻⁶ g(1)/100 g sln and
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure-	.55 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS:
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by	.55 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole %
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene	.55 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY ÆTHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt	.55 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ -
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY ETHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther-	.55 x 10 ⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO ₄ -
Calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed</pre>
Calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR:</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter employed a ratio-photon counting	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 4.3 % (author)</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure-	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR:</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter employed a ratio-photon counting mode where anthracene concentration was linearly related to the fluore- scence signal. The UV method was	<pre>INFORMATION INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 4.3 % (author) Temperature ± 0.1°C (author)</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter employed a ratio-photon counting mode where anthracene concentration was linearly related to the fluore- scence signal. The UV method was used to obtain the absorptivity of	<pre>.55 x 10⁻⁶ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 4.3 % (author)</pre>
calculated by the compilers are 3. 3.69 x 10 ⁻⁹ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of anthracene in NaCl solution was determined by fluore- scence and UV absorption measure- ments. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluor- escence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a ther- mostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter employed a ratio-photon counting mode where anthracene concentration	<pre>INFORMATION INFORMATION SOURCE AND PURITY OF MATERIALS: Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex column. ESTIMATED ERROR: Solubility ± 4.3 % (author) Temperature ± 0.1°C (author)</pre>

50_557	407
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Anthracene; C ₁₄ H ₁₀ ; [120-12-7]	May, W.E.; Wasik, S.P.; Freeman D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of anthracene in aque	ous sodium chloride is
reported in terms of the Setschenow e	equation:
$\log(S_{o}/S) = K_{s}C_{s}$	
where;	
S _o is the solubility of	of (1) in water (mg/L)
S is the solubility of	f (l) in saline solution (mg/L)
K _s is the Setschenow of	constant (L/mol)
C _s in the concentratio	on of sodium chloride (mol/L)
evaluating the equation for S over the	ne range of C _s 0-0.7 (mol/L)
$K_{s} = 0.238$ with $S_{o} = 0.0446$.	-
The corresponding mass percent and mo	ble fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the comp	pilers are 3.11 x 10 ⁻⁶ g(1)/kg sln
and 3.22×10^{-9} .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The saturated solution was extracted	(3) distilled from potassium permanganate-sodium hydroxide
with an "extractor column" packed	and passed through an XAD-2
with a superficially porous bonded C_{18} stationary phase, then a water-	column.
ačetonitrile solvent was passed	
through for extraction. The extract was introduced into a	
liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a UV detector.	temp ± 0.05°C K _s ± 0.004
	s ± 0.0002
	REFERENCES:

COMPONENTS: EVAI	ALUATOR:
(2) Water; H ₂ O; [7732-18-5] and Uni	T. Hefter, School of Mathematical d Physical Sciences, Murdoch iversity, Perth, W.A., Australia. bruary 1986.

Quantitative solubility data for phenanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported for the solubility of water in phenanthrene.

TABLE 1: Quantitative Solubility Studies of Phenanthrene (1) in Water (2)			
Reference	T/K	Method	
Davis et al. (ref 1)	300	nephelometric	
Andrews and Keefer (ref 2)	298	spectrophotometric	
Klevens (ref 3)	298	spectrophotometric	
Wauchope and Getzen (ref 4)	273-348	spectrophotometric	
Eganhouse and Calder (ref 5)	298	GLC	
Mackay and Shiu (ref 6)	298	spectrofluorometric	
Schwarz (ref 7)	282-305	spectrofluorometric	
May et al. (ref 8)	282-303	chromatographic	

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

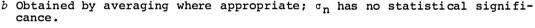
The plethora of values reported (Table 1) at 298K for the solubility of phenanthrene (1) in water (2) enable a particularly critical assessment to be made. Thus the values of Davis *et al*. (ref 1) at 300K and of Klevens (ref 3) have been rejected as they are significantly higher than all other values. The remaining data at 298K are in good agreement enabling the average value to be Recommended.

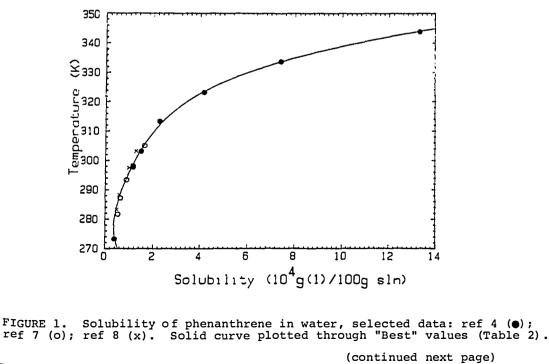
At other temperatures where comparison is possible the data of May *et al.* (ref 8), Schwarz (ref 7) and Wauchope and Getzen (ref 4) are in excellent agreement enabling the average values to be Recommended over a reasonably wide range. At higher temperatures (> 303K) only the data of Wauchope and Getzen (ref 4) are available and must therefore be regarded as Tentative.

All the available data, except for the rejected values noted above (ref 1, 3), are summarized in Table 2 and plotted in Figure 1.

COMPONENT	TS:	VALUATOR:
	ter; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. Pebruary 1986.
CRITICAL	EVALUATION: (continued)	
	TABLE 2: Recommended (R) and 7 Phenanthrene (1)	
<i>Т/</i> К	Solubility values	
	Reported values ^a 10 ⁴ g(1)/100g sln	"Best" values $(\pm \sigma_n)^b$ 10 ⁴ g(1)/100g sln 10 ⁷ x_1
273	0.39 (ref 4)	0.4 0.4
283	0.53* (ref 7), 0.46* (ref 8)	$0.50 \pm 0.04 (R)$ $0.50 (R)$
29 3	0.88* (ref 7), 0.78* (ref 8)	0.85 ± 0.05 (R) 0.86 (R)
298	0.994 (ref 2), l.18 (ref 4), l.07 (ref 5), l.29 (ref 6), l.151 (ref 7), l.002 (ref 8)	
303	l.50* (ref 4), l.46* (ref 7) l.28* (ref 8)	, 1.4 ± 0.1 (R) 1.4 (R)
313	2.45* (ref 4)	2.5 2.5
323	4.14 (ref 4)	4.1 4.1
333	7.2* (ref 4)	7.2 7.2
343	12.8* (ref 4)	13 13
515	17 (ref 4)	17 17

graphical interpolation of the authors' original data. b Obtained by averaging where appropriate; σ_n has no statistical signifi-





EVALUATOR: COMPONENTS: (1) Phenanthrene; C₁₄H₁₀; [85-01-8] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. February 1986. (continued) CRITICAL EVALUATION: REFERENCES Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1942, 64, 1. 108-10. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-77. 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-298. з. 4. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data 1972, 17, 38-41. 5. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40, 555-61. 6. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7. 7. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-8. 1000. ACKNOWLEDGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Water; H₂0; [7732-18-5]</pre>	<pre>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.</pre>
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of phe	nanthrene in water
t/°C	$10^3 g(1) L^{-1} (2)$
27	1.55
	1.65
The best value recommended by the aut Assuming that 1.00 L sln = kg sln t mole fraction, x_1 , calculated by the 100 g sln and 1.62 x 10^{-7} .	he corresponding mass percent and
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) Eastman Kodak Company, 599; m.p. range 100.0-100.9°C; used as received; (cf. ref 2). (2) dust-free.
	ESTIMATED ERROR:
	temp. \pm 3°C soly. \pm 0.05 x 10 ⁻³ g(1) dm ⁻³ (2)
	REFERENCES:
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

412	38_340	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Andrews, L.J.; Keefer, R.M.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES:		
The solubility of phenanthrene in water at 25°C was reported to be 9.94 x 10^{-5} g(1)/100 g sln. The corresponding mole fraction, x_1 , value calculated by compiler is 1.004 x 10^{-7} .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a mea-	 (1) Eastman Kodak Co., best grade; recrystallized twice from ethanol; m.p. 101.0°C. (2) not specified. 	

ESTIMATED ERROR:

sured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorb-ance of the hexane phase was mea-

sured against a hexane blank on the

Beckman spectrophotometer.

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

The solubility phenanthrene in water at 25°C was reported to be 0.0016 x 10^{-5} /L sln and 9.0 x 10^{-6} mole (1)/L sln. Assuming that 1.00 dm³ sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.6 x 10^{-4} g(1)/100 g sln and 1.62 x 10^{-7} .

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski

.

EXPERIMENTAL VALUES:

		ity of phenanthr		
	mg(l)/kg(2)	. 4 (1) (100 1	$10^{7}x_{1}$
t/°C		smoothed with	10^4 g(l)/100 g sln	
	experiment	(std dev)	(compiler)	(compiler)
0.0		0.39(0.01)	0.39	0.39
24.6	1.12, 1.11	1.16	1.16	1.17
25.0	·	1.18(0.02)	1.18	1.19
29.9	1.49, 1.49	1.49	1.49	1.51
30.3	1.47, 1.48	1.52	1.52	1.54
38.4		2.27	2.27	2.29
40.1	2.27, 2.28, 2.25	2.47	2.47	2.50
47.5	3.81, 3.88, 3.87	3.63	3.63	3.67
50.0		4.14(0.04)	4.14	4.18
50.1	4.30, 4.38, 4.32	4.16	4.16	4.20
50.2	4.08, 4.04, 4.11	4.19	4.19	4.23
54.7	5.66, 5.64, 5.63	5.34	5.34	5.40
59.2	7.17, 7.19, 7.21	6.85	6.85	6.92
60.5	7.2, 7.2, 7.6	7.4	7.4	7.5
65.1	9.8, 9.7, 9.8	9.6	9.6	9.7
70.7	12.4, 12.6, 12.4	13.3	13.3	13.4
71.9	12.9	14.2	14.2	14.4
73.4	18.2	15.6	15.6	15.8
75.0		17.2(0.3)	17.2	17.4

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The	SOURCE AND PURITY OF MATERIALS: (1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice;
flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete	purity not specified. (2) distilled and deionized.
extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glass-	ESTIMATED ERROR: temp. ± 0.5°C soly. see experimental values above
ware.	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Water; H₂0; [7732-18-5]</pre>	Eganhouse, R.P.; Calder, J.A. <i>Geochim. Cosmochim. Acta</i> <u>1976</u> , 40, 555-61.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of phenanthrene in water at 25°C was reported to be 1.07 mg(1)/kg(2) and 6 x 10^{-6} mol(1) dm ⁻³ (2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.07 x 10^{-4} g(1)/100 g sln and 1.08 x 10^{-7} .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:		
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detec- tors was employed.	<pre>(1) source not specified; analytical grade; used as</pre>	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Mackay, D.; Shiu, W.Y.	
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of phenanthrene in water at 25°C was reported to be 1.29 mg(1) dm ⁻³ sln and $x_1 = 1.3 \times 10^{-7}$. The corresponding mass percent calculated by the compiler is 1.29 x 10 ⁻⁴ g(1)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.07 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES: </pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Water; H ₂ O; [7732-18-5]	Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.4-31.8°C	A. Maczynski

EXPERIMENTAL VALUES:

	Solubility of phe	nanthrene in water	
<i>t</i> /°C	10 ⁶ mol(1) L ⁻¹	<pre>10⁵ g(1)/100 g sln</pre>	10 ⁸ x1 (compiler)
8.4	2.81 ± 0.07	5.01	5.06
11.1	3.09 ± 0.07	5.51	5.57
14.0	3.59 ± 0.06	6.40	6.47
17.5	4.40 ± 0.04	7.84	7.92
20.2	4.94 ± 0.09	8.80	8.90
23.3	6.09 ± 0.07	10.85	10.97
25.0	6.46 ± 0.02	11.51	11.63
29.3	7.7 ± 0.2	13.72	13.87
31.8	9.13 ± 0.08	16.27	16.44

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Two methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures.	 SOURCE AND PURITY OF MATERIALS: (1) source not specified; better than 99 mole%, by glc; used as received. (2) distilled over KMnO₄ and NaOH and passed through a Sephadex
At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above
	REFERENCES :

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418			38_340	
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]		May, W.E.; Wasik, S.P.; Freeman, D.H.		
(2) Water; H ₂ O; [7732-18-5]		Anal. Chem. <u>1978</u> , 50, 175-9 and 997-1000.		
VARIABLES:		PREPARED BY:		
Temperature: 8.5-29.9°C A. Maczynski				
EXPERIMENTAL VA	LUES:			
	Solubility of p	nenanthrene in water		
t/°C	μg(l)/kg(2)	10 ⁴ g(1)/100 g sln (compiler)	10 ⁸ x1 (compiler)	
8.5	423 ± 4	0.423	0.427	
10.0	468 ± 2	0.468	0.473	
12.5	512 ± 1	0.512	0.517	
15.0	601 ± 7	0.601	0.607	
21.0	816 ± 8	0.816	0.825	
24.3	995 ± 1	0.995	1.006	
25.0	1002 ± 11	1.002	1.013	
29.0	1220 ± 13	1.220	1.233	
29.9	1277 ± 11	1.277	1.291	
	AUXILIARY	INFORMATION		
METHOD/APPARATU	JS/PROCEDURE:	SOURCE AND PURITY OF MATERI	ALS:	
chromatograp	coupled column liquid phy (DCCLC) method was nerating saturated solu-	(1) commercial product than 3% impurities		
tions by pur column packed have been co (1) (generation centration of the generation sured by a r	mping water through a ed with glass beads that bated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato-	(2) distilled over KMr and passed through packed with XAD-2 Hass, Philadelphia	n a column (Rohm and	
graphic pro	cess that has been	ESTIMATED ERROR:		
described in	n ref l.	temp. ± 0.05°C soly. stand. dev. see	above	
		REFERENCES: 1. May, W.; Chesler, S Gump, B.; Hertz, H. Dyszel, S. J. Chro 1975, 13, 535.	; Enagonio, D.:	

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COMPONENTS :	EVALUATOR:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

The solubility of phenanthrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Method	Salinity g salts/kg sln	10 ⁵ g(1)/100 g sln
Eganhouse and Calder (ref 1)	GLC	35	7.1
Schwarz (ref 2)	v spectral	30	9.94
May et al. (ref 3)	HPLC	35	6.63
Aquan-Yuen et al. (ref 4) u	v spectral	28.6	8.3

At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder and of May *et al*. are in very good agreement. Therefore their mean, 6.9×10^{-5} g (1)/100 g sln is adopted as the recommended value for the solubility of phenanthrene at the indicated temperature and salinity. The value of Aquan-Yuen *et al*. appears consistent with the data discussed above and with the recommended value for the solubility of phenanthrene in pure water and is adopted at tentative. The value of Schwarz appears slightly high and is considered doubtful.

	THE SOLUBILITY C	DF PHENANTHRENE (1) RECOMMENDED VALUE	IN SEAWATER (2)
т/к		g salts/kg sln	10 ⁵ g(1)/100 g sln
298		35	6.9

REFERENCES

- Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u>, 40, 555-61.
- 2. Schwarz, F.P. J. Chem. Eng. Data <u>1977</u>, 22, 273-7.
- 3. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.
- 4. Aquan-Yuen, M.; Mackay, D.; Shui, W.Y. J. Chem. Eng. Data <u>1979</u>, 24, 30-4.

420	38_348
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Artificial seawater (ref. 1)</pre>	Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta <u>1976</u> , 40, 555-61.
VARIABLES: One temperature: 25.0°C Salinity: 35 g/kg sln EXPERIMENTAL VALUES: The solubility of phenanthrene in sear the corresponding mass percent and mo the compilers are 7.1 x 10 ⁻⁵ g(1)/100 Graphical results for other salinities	le fraction, x_1 , calculated by g sln and 7.4 x 10^{-8} .
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Equilibrium flask: 1-dm ³ Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agita- ted 12+ hr at 215 rpm on a New Bruns- wick gyrotary shaker; a 24 hr sta- tionary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard. Analysis: gas chromatography.	<pre>SOURCE AND PURITY OF MATERIALS: (1) analytical grade salt for artificial seawater solution, reagent grade. Water: doubly distilled. ESTIMATED ERROR: temperature: ± 0.5°C soly: ± 0.025 (95% confidence interval) REFERENCES: 1. Lyman, J.; Fleming, R.H.; J. Mar. Res. 1940, 3, 135.</pre>

COMPONENTS:	
	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8]	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 11.1 - 31.8°C	W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	
EXPERIMENTAL VALUES:	
Solubility of phenanthrene	in 0.5 mol(2)/L
<u>t/°C</u> <u>10⁶ m</u>	ol(1)/L sln
	88
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
20.2 4.	51
23.2 5. 25.0 5.	
29.3 7.	2
31.8 7.	9
25.0°C calculated by the co sln and 1.034 x 10 ⁻⁷ .	mpilers are 9.94 x 10 ⁻⁵ g(l)/100 g
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of phenanthrene was	
determined by fluorescence and UV absorption measurements. For fluor-	Phenanthrene: purity 99.9%
	Phenanthrene: purity 99.9% Sodium chloride: reagent grade
escence method, an excess amount of	Sodium chloride: reagent grade
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ -
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column.
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra-	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author)
escence method, an excess amount of phenanthrene was added to an air- tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solu- tion. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentra- tion was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence	Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 8.4% (author) Temperature ± 0.1°C (author)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]	May, W.E.; Wasik, S.P.; Freeman,
	D. H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	W. Y. Chin and D. Mackau
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of phenanthrene in aq in terms of the Setschenow equation:	ueous sodium chloride is reported
$\log(S_{o}/S) = K_{s}C_{s}$	
where;	
S _o is the solubi	lity of (l) in water (mg/L)
S is the solubil	ity of (1) in saline solution (mg/L)
K_ is the Setsch	enow constant (L/mol)
5	tration of sodium chloride (mol/L)
evaluating the equation for S over t	
$K_{s} = 0.275$ with $S_{o} = 1.002$.	s s s s s s s s s s s s s s s s s s s
s 0.275 with 0 1.002.	
The corresponding mass percent and m	ole fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the com	pilers are 6.63 x 10^{-5} g(l)/100 g sln
and 6.78×10^{-8} .	
Graphical data for other temperature	s are also presented.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was prepared by pumping salt water	(1) greater than 97% pure.
through a "generation column" which was packed with glass beads coated	(2) reagent grade.
with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	Permanganate-sodium hydroxide and passed through an XAD-2
with a superficially porous bonded C_{18} stationary phase, then a water-	column.
acetonitrile solvent was passed through for extraction. The	
extract was introduced into a	
liquid chromatograph and the concen- tration of (1) was measured with a	temp ± 0.05°C
UV detector.	$ \begin{array}{c} K & \pm & 0.010 \\ S_0^{S} & \pm & 0.011 \end{array} $
	REFERENCES :

<pre>(1) Phenanthrene; C₁₄H₁₀; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H₂O; [7732-18-5] VARIABLES: One temperature: 25°C Salinity: 29-108 g(2)/kg sln EXPERIMENTAL VALUES: Solubility of phenanth</pre>	Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1979</u> , 24, 30-4. PREPARED BY: M. Kleinschmidt and W. Shiu
	(1)/L sln 10^5 mass $(1)^a$ $10^8 x_1^a$
0.50 28.6 1.00 56.2 1.50 82.6 2.00 108.2	0.85 8.3 8.6 0.67 6.4 6.8 0.48 4.5 4.9 0.33 3.1 3.3
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Saturated solutions were prepared by adding excess (1) to a pre- viously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectro- fluorometrically.	<pre>SOURCE AND PURITY OF MATERIALS: (1) fluorescence grade, from Eastman Kodak. (2) reagent grade, from Fisher Scientific. ESTIMATED ERROR: temp ± 0.5°C soly ± 3 relative % REFERENCES: 1. Weast, R.C.; CRC Handbook of Chemistry and Physics, 59th Edition; 1978; CRC Press pp. D299-D300.</pre>

ORIGINAL MEASUREMENTS:

COMPONENTS:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) (E)-Stilbene; C ₁₄ H ₁₂ ; [103-30-3]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1950</u> , 72, 5034-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of (E)-stilbene in wat to be 2.9 x 10 ⁻⁵ g(l)/100 g sln.	ter at 25°C was reported
The corresponding mole fraction, x_1 , is 2 x 10^{-8} .	calculated by the compilers
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a	(1) from the State University of Iowa;
constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous	m.p. 120-121°C;
phase was withdrawn and extracted with a measured volume of hexane	(2) not specified.
(10-50 mL) by shaking in a glass- stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase	
was measured against a hexane blank on the Beckman spectrophotometer.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

30_333	425
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1,4-Dicyclopentylbutane; C ₁₄ H ₂₆ ; [2980-70-3]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Technol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in 3	l,4-Dicyclopentylbutane
<u>t/°C</u> g(2)/100 g s	$\ln \frac{10^3 x_2 (compiler)}{1}$
10 0.0088 20 0.0139 30 0.0241	0.94 1.50 2.59
30 0.0241	2.59
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated	(1) Not specified.
for 5 hr. with (2). Next, calcium hydride was added and the evolving	(2) Not specified.
hydrogen volume measured and hence the concentration of (2) in (1) was	
evaluated.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	REFERENCES:
	I

COMPONENTS:	EVALUATOR:
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

Quantitative solubility data for the tetradecane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe Tetradecane (1) - Water (2) System

Reference	Т /К	Solubility	Method
Schatzberg (ref 1)	313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC
Mackay et al. (ref 4)	_ a	(1) in (2)	GLC

a Not specified but probably close to 298 K.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF TETRADECANE (1) IN WATER (2)

The solubility of tetradecane in water has been reported only at 298K (Table 1). Unfortunately, the results are in very poor agreement (Table 2). Furthermore, all the reported values are very much higher than the value of $\sim 3 \times 10^{-8}$ g(1)/100 g sln which is predicted by extrapolation of the lower hydrocarbon homologue solubilities. Thus, the values given in Table 2 must be regarded very sceptically and no "Best" value has been calculated.

TABLE 2:	Reported Solubility Values of
Tetr	adecane (1) in Water (2)
	<i>q</i>
	Reported solubility values ^a
	$10^7 g(1)/100 g sln$

298

T/K

6.94 (ref 2), 2.2 (ref 3), 25.9^b (ref 4)

a All values may be high. "Best" values not determined because of uncertainties in data, see text.

b Assumed to be at 298K for the purpose of comparison.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN TETRADECANE

As only the datum of Schatzberg at 313K is available no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the appropriate Data Sheet for the experimental value.

REFERENCES

- 1. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.
- 2. Franks, F. Nature (London) <u>1966</u>, 210, 87-8.
- 3. Sutton, C.; Calder, J.A. Environ. Sci. Technol. 1974, 8, 654-7.
- Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u>, 573, 251-8.

HWW 2-CC

428	38_355
COMPONENTS: (1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5] VARIABLES: One temperature: 40°C EXPERIMENTAL VALUES: The solubility of water in tetradecan 114 mg(2)/kg sln corresponding to a m	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: (1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and com- pletely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorp- tion occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. 0-2% (deviations from the mean) REFERENCES:</pre>

38_356	429
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Tetradecane; H ₁₄ H ₃₀ ; [629-59-4]	Franks, F.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1966</u> , 210, 87-8.
	•
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of tetradecane in wate	er at 25°C was reported to be
in mole fraction $x_1 = 6.3 \times 10^{-10}$.	
The corresponding mass percent calcul 6.94×10^{-7} g(1)/100 g sln.	ated by the compiler is
6.94 x 10 g(1)/100 g sin.	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chroma- tographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.	 (1) Fluka; purum grade; purity > 97% (chromatographic analysis). (2) not specified. ESTIMATED ERROR:			
	soly. ± 12%			
	REFERENCES:			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	Sutton, C.; Calder, J.A.		
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The solubility of tetradecane in wate 2.2 x 10 ⁻⁷ g(1)/100 g(2) correspondin 2 x 10 ⁻¹⁰ .			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	<pre>(1) Analabs Inc., 99+%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:</pre>		

	المحمد المحمد المحمد والمحمد فللتعاد والمحمد فالمحمد المحمد المحمد والمحمد المحمد المحمد المحمد المحمد المحمد ا			
COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Water; H ₂ O; [7732-18-5]	<pre>Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, 573, 251-8.</pre>			
VARIABLES:	PREPARED BY:			
not specified	M.C. Haulait-Pirson			
EXPERIMENTAL VALUES:				
The authors reported a value of 0.0259 mg(1)dm ⁻³ sln for the solubility of tetradecane in water. With the assumption of a solution density of 1.00 g cm ⁻³ the corresponding mass percent, calculated by the compiler, is 2.59 x 10^{-6} g(1)/100 g sln and the corresponding mole fraction, x_1 , is 2.4 x 10^{-9} .				

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;			
(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equili- brations it is possible to calculate the amount of (1) in the original sample.	ESTIMATED ERROR:			
	not estimated.			
	REFERENCES :			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Seawater	Sutton, C.; Calder, J.A. <i>Environ. Sci. Technol.</i> <u>1974</u> , 8, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	PREPARED BY: P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of tetradecane in seawater was reported to be 1.7 x 10^{-7} g(1)/100 g sln and $x_1 = 1.5 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
METHOD/APPARATUS/PROCEDURE: (1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^{\circ}$ C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	Analabs, Inc., North Haven, Conn.		
	ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.		
	REFERENCES:		

COMPONENTS:	EVALUATOR:
 (1) 2-Methylanthracene; C₁₅H₁₂; [613-12-7] (2) Water; H₂O; [7732-18-5] 	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

Quantitative solubility data for 2-methylanthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2-methylanthracene.

TABLE 1:	Quantitative	Solub	ility	Stu	dies	of
2-Me	thylanthracene	e (1)	in Wa	ter	(2)	

Reference	Т /К	Method
Mackay and Shiu (ref 1)	298	spectofluorometric
May <i>et al</i> . (ref 2)	279-304	chromatographic

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

At 298K, the only temperature at which comparison is possible, the datum of Mackay and Shiu (ref 1) is in only fair agreement with that of May *et al.* (ref 2). Thus all the available data, which are summarized in Table 2, must be regarded as very tentative.

TABLE 2: Tentative Solubility Values of 2-Methylanthracene (1) in Water (2)

Т /К	Solubility values		
	Reported values ^{a}	"Best values ($(\pm \sigma_n)^b$
	10 ⁶ g(1)/100 g sln	10 ⁶ g(1) g sln	$10^9 x_1$
278	0.64* (ref 2)	0.6	0.6
283	0.89* (ref 2)	0.9	0.8
293	1.60* (ref 2)	1.6	1.5
298	3.9 (ref 1), 2.16* (ref 2)	3.0 ± 0.9	2.8
303	2.93 (ref 2)	3.0	2.8

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

REFERENCES

1. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

2. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 2-Methylanthracene; C₁₅H₁₂; 	Mackay, D.; Shiu, W.Y.
[613-12-7]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
VARIABLES:	PREPARED BY:
TANIADESS	TREFARED DI.
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 2-methylanthracene	in water at 25°C was reported
to be 0.039 mg(1) dm ⁻³ sln and $x_1 = 3$	
The corresponding mass percent calcul	stad by the compiler
is 3.9×10^{-6} g(1)/100 g sln.	ated by the compiler
	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2)	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL	Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was decanted and filtered and 50-100 mL	
extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory funnel. After shaking for 2 hrs.	
the cyclohexane extract was removed for analysis. An Aminco-Browman	
spectrophotofluorometer (American	1
Instruments Ltd.) was used for analysis. Many details are given	ESTIMATED ERROR: soly. \pm 0.004 mg(l) dm ⁻³ sln
in the paper.	(maximum deviation from several
	determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2-Methylanthracene; C ₁₅ H ₁₂ ;	May, W.E.; Wasik, S.P.; Freeman, D.H.	
[613-12-7]	Anal. Chem. 1978, 50, 175-9 and	
(2) Water; H ₂ O; [7732-18-5]	997-1000.	
VARIABLES:	PREPARED BY:	
Temperature: 6.3-31.1°C	A. Maczynski	
EXPERIMENTAL VALUES:		
Solubility of 2-methy	lanthracene in water	
t/°C μg(1)/kg(2)	$10^{6} g(1)/100 g sln 10^{9} x_{1}$	
	(compiler) (compiler)	
6.3 7.06 ± 0.18	0.706 0.661	
9.1 8.48 ± 0.09	0.848 0.794	
10.8 9.43 ± 0.37	0.943 0.883	
13.9 11.1 ± 0.3	1.11 1.04	
18.3 14.5 ± 0.1	1.45 1.36	
23.1 19.1 ± 0.6	1.91 1.79	
25.0 21.3 ± 0.3	2.13 1.99	
27.0 24.2 ± 0.1	2.42 2.27	
31.1 32.1 ± 0.3	3.21 3.01	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The dynamic coupled column liquid chromatography (DCCLC) method was	<pre>(1) commercial product; less than 3% impurities.</pre>	
based on generating saturated solu-		
tions by pumping water through a column packed with glass beads that	(2) distilled over KMnO ₄ and NaOH and passed through a column	
have been coated with the component	packed with XAD-2 (Rohm and	
(1) (generator column). The con- centration of (1) in the effluent	Hass, Philadelphia, Pa).	
of the generator column was mea-		
sured by a modification of the coupled column liquid chromato-		
graphic process that has been described in ref 1.	ESTIMATED ERROR:	
	temp. ± 0.05°C soly. stand. dev. see above	
	REFERENCES:	
	<pre>1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.</pre>	
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38_362

430	38_363
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Methylanthracene; C₁₅H₁₂; [613-12-7]</pre>	May, W.E.; Wasik, S.P.; Freeman D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997 - 1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of 2-methylanthracene	in aqueous sodium chloride is
reported in terms of the Setschenow e	equation:
$\log(S_{o}/S) = K_{S}C_{S}$	
where;	
S _o is the solubility o	of (1) in water (mg/L)
S is the solubility of	(1) in saline solution (mg/L)
K _c is the Setschenow of	constant (L/mol)
5	on of sodium chloride (mol/L)
evaluating the equation for S over th	
$K_{\rm s} = 0.336$ with $S_{\rm o} = 0.0213$.	S S
The corresponding mass percent and mo	ble fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the comp	oilers are 1.29 x 10 ⁻⁶ g(1)/100 g sln
and 1.24×10^{-9} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2
with a superficially porous bonded C_{10} stationary phase, then a water-	column.
acetonitrile solvent was passed	
through for extraction. The extract was introduced into a	
liquid chromatograph and the concen- tration of (1) was measured with a	ESTIMATED ERROR: temp ± 0.05°C
UV detector.	$K_{s} \pm 0.006$
	S ₀ ± 0.003
	REFERENCES :

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38_364	437
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 9-Methylanthracene; C ₁₅ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[779-02-2]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 9-methylanthracene to be 0.261 mg(1) dm ⁻³ sln and $x_1 = 2$ The corresponding mass percent calcul is 2.61 x 10 ⁻⁵ g(1)/100 g sln.	2.44×10^{-8} .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.002 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES: </pre>

/1		ORIGINAL MEASUREMENTS:	
(1) 1-Methyl	lphenanthrene; C ₁₅ H ₁₂ ;	May, W.E.; Wasik, S.P.	; Freeman, D.H.
[832-69-6]		Anal. Chem. <u>1978</u> , 50	, 175-9 and
(2) Water; H	H ₂ 0; [7732-18-5]	997-1000.	
VARIABLES:		PREPARED BY:	
Temperature	: 6.6-29.9°C	A. Maczynski	
-			
EXPERIMENTAL VA	LUES:		
	Solubility of 1-methy	lphenanthrene in water	
t/°C	μg(l)/kg(2)	10 ⁵ g(1)/100 g sln (compiler)	10 ⁸ x1 (compiler)
6.6	95.2 ± 0.2	0.952	0.892
8.9	114.0 ± 4.0	1.14	1.07
14.0	147.0 ± 1.0	1.47	1.38
19.2	193.0 ± 1.0	1.93	1.81
24.1	255.0 ± 5.0	2.55	2.39
25.0	269.0 ± 3.0	2.69	2.69
26.9	304.0 ± 1.0	3.04	2.85
29.9	355.0 ± 2.0	3.55	3.32
	AUXILIARY	INFORMATION	
METHOD/APPARATU		INFORMATION SOURCE AND PURITY OF MATERI	TALS:
The dynamic	US/PROCEDURE: coupled column liquid	SOURCE AND PURITY OF MATERI	t; less
The dynamic chromatograp	US/PROCEDURE: coupled column liquid phy (DCCLC) method was	SOURCE AND PURITY OF MATERI	t; less
The dynamic chromatograp based on gen tions by pur	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a	SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KM	t; less s. nO4 and NaOH
The dynamic chromatograp based on gen tions by pur column packe	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that	SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KM and passed through	t; less s. nO4 and NaOH h a column
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generat	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con-	SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KM	t; less s. nO4 and NaOH h a column (Rohm and
The dynamic chromatograp based on gen tions by pur column packa have been co (1) (generation of	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent	 SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KM and passed through packed with XAD-2 	t; less s. nO4 and NaOH h a column (Rohm and
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generation of the generation sured by a n	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the	 SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KM and passed through packed with XAD-2 	t; less s. nO4 and NaOH h a column (Rohm and
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generation (1) (generation centration of the generation sured by a re coupled colu	US/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea-	 SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KMA and passed throug packed with XAD-2 Hass, Philadelphi 	t; less s. nO4 and NaOH h a column (Rohm and
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generation (1) (generation of the generation sured by a r coupled colu	JS/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato- cess that has been de-	<pre>SOURCE AND PURITY OF MATERI (1) commercial product than 3% impurities (2) distilled over KM and passed through packed with XAD-2 Hass, Philadelphis ESTIMATED ERROR:</pre>	t; less s. nO4 and NaOH h a column (Rohm and
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generation of the generation of the generation sured by a re coupled colu- graphic prod	JS/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato- cess that has been de-	 SOURCE AND PURITY OF MATERI (1) commercial production than 3% impurities (2) distilled over KMA and passed throug packed with XAD-2 Hass, Philadelphi 	t; less s. nO ₄ and NaOH h a column (Rohm and a, Pa).
chromatograp based on gen tions by pur column packe have been co (1) (generation of the generation sured by a re coupled colu- graphic proc	JS/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato- cess that has been de-	<pre>SOURCE AND PURITY OF MATERI (1) commercial product than 3% impurities (2) distilled over KM and passed throug packed with XAD-2 Hass, Philadelphis ESTIMATED ERROR: temp. ± 0.05°C</pre>	t; less s. nO ₄ and NaOH h a column (Rohm and a, Pa).
The dynamic chromatograp based on gen tions by pur column packe have been co (1) (generation of the generation sured by a re coupled colu- graphic proc	JS/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato- cess that has been de-	<pre>SOURCE AND PURITY OF MATERI (1) commercial product than 3% impurities (2) distilled over KM and passed through packed with XAD-2 Hass, Philadelphin ESTIMATED ERROR: temp. ± 0.05°C soly. stand. dev. see</pre>	t; less s. nO ₄ and NaOH h a column (Rohm and a, Pa). above S.; Cram, S.; .; Enagonio, D.
The dynamic chromatograp based on gen tions by pur column pack have been co (1) (generation of the generation sured by a r coupled colu- graphic prod	JS/PROCEDURE: coupled column liquid phy (DCCLC) method was nerating saturated solu- mping water through a ed with glass beads that oated with the component tor column). The con- of (1) in the effluent rator column was mea- modification of the umn liquid chromato- cess that has been de-	<pre>SOURCE AND PURITY OF MATERI (1) commercial product than 3% impurities (2) distilled over KM and passed through packed with XAD-2 Hass, Philadelphis ESTIMATED ERROR: temp. ± 0.05°C soly. stand. dev. see REFERENCES: 1. May, W.; Chesler, Soly. Stand. dev. see REFERENCES: 1. May, W.; Chesler, Soly. Stand. St</pre>	t; less s. nO ₄ and NaOH h a column (Rohm and a, Pa). above s.; Cram, S.; .; Enagonio, D.

38_300	439	
COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) 1-Methylphenanthrene; C₁₅H₁₂; [832-69-9]</pre>	May, W.E.; Wasik, S.P.; Freeman, D.H.	
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.	
(3) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 25°C		
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay	
EXPERIMENTAL VALUES:		
The solubility of 1-methylphenanthrene in aqueous sodium chloride is		
reported in terms of the Setschenow	equation:	
$\log(S_{O}/S) = K_{S}C_{S}$		
where;		
S _o is the solubility	of (1) in water (mg/L)	
S is the solubility o	f (1) in saline solution (mg/L)	
K _s is the Setschenow	constant (L/mol)	
C ₂ in the concentrati	on of sodium chloride (mol/L)	
evaluating the equation for S over t	he range of $C_0 - 0.7 \text{ mol/L}$,	
$K_{\rm s} = 0.211$ with $S_{\rm o} = 0.269$.		
The corresponding mass percent and mole fraction x_1 , at salinity =		
35 g(2)/kg sln calculated by the compilers are 1.95 x 10^{-5} g(1)/100 g sl		
and 1.87 $\times 10^{-8}$.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
A saturated solution of (1) was	(1) greater than 97% pure.	
prepared by pumping salt water through a "generation column" which	(2) reagent grade.	
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium	
saturated solution was extracted	permanganate-sodium hydroxide and passed through an XAD-2	
with an "extractor column" packed with a superficially porous bonded	column.	
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed		
through for extraction. The extract was introduced into a	ESTIMATED ERROR:	
liquid chromatograph and the concen- tration of (1) was measured with a	$temp \pm 0.05^{\circ}C$	
UV detector.	$K \pm 0.018$ $S_0^{s} \pm 0.003$	
	REFERENCES:	

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COMPONENTS:	EVALUATOR:
<pre>(1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

Quantitative solubility data for fluoranthene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in fluoranthene.

TABLE 1. Quantitative Solubility Studies of Fluoranthene (1) in Water (2)		
Reference	Т / К	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. They are also summarized in Table 2. The values at 298 K are in reasonable agreement given the low solubility and the average value is Recommended. The remaining data are regarded as Tentative only.

TABLE 2. Recommended (F) and Tentative Solubility Values of Fluoranthene (1) in Water (2)

Т /К	Solubility values			
	Reported values 10 ⁵ g(l)/100 g sln	"Best" values $(\pm \sigma_n)^a$ 10 ⁵ g(1)/100 g sln 10 ⁸ x_1		
298	2.65 (ref 2), 2.6 (ref 3), 2.06 (ref 4)	2.4 ± 0.3 (R) 2.1 (R)		
300	2.40 (ref 1)	2.4 2.1		
302	2.64 (ref 4)	2.6 2.3		

a Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. <u>1950</u>, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Fluoranthene; C₁₆H₁₀; [206-44-0] (2) Water; H₂0; [7732-18-5]</pre>	<pre>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.</pre>
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES:			
Solubility of flu t/°C	oranthene in water 10^4 g(1) L ⁻¹ (2)		
27	2.40 ± 0.20 2.25 ± 0.20 2.40 ± 0.20		
The best value recommended by the authors is 2.40 x 10^{-4} g(1) L ⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction are 2.40 x 10^{-5} g(1)/100 g sln and 2.15 x 10^{-8} .			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) prepared at Harvard University; m.p. range 110.0-110.7°C; (cf. ref 2). (2) dust-free. 		
	ESTIMATED ERROR: temp. ± 3°C soly. see above		
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	•

The solubility of fluoranthene in water at 25°C was reported to be 2.65 x 10^{-4} g(1) L⁻¹ and 1.32 x 10^{-6} mole/L⁻¹. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 2.65 x 10^{-5} g(1)/100 g sln and 2.37 x 10^{-8} .

AUXTLTARY	INFORMATION	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:
	l

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of fluoranthene in wat to be 0.26 mg(1) dm ⁻³ sln and $x_1 = 2$. The corresponding mass percent calcul	28×10^{-8} .
is 2.6 x 10^{-5} g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American	 (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled.
Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. ± 0.002 mg(l) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Fluoranthene	e; C H :	May, W.E.; Wasik, S.P.	; Freeman, D.H.
[206-44-0]	, c ₁₆ 10,	Anal. Chem. 1978, 50,	
(2) Water; H ₂ O;	[7732-18-5]	<u><u> </u></u>	
VARIABLES:		PREPARED BY:	
Temperature: 25	and 29°C	A. Maczynski	
EXPERIMENTAL VALUES:			
			}
	Solubility of fluor	ranthene in water	
<i>t/°</i> C	mg(l)/kg(2)	10 ⁵ g(1)/100 g sln (compiler)	10 ⁸ x1 (compiler)
25	0.206	2.06	1.83
29	0.264	2.64	2.35
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PRO		SOURCE AND PURITY OF MATERIA	[
chromatography based on generat tions by pumping column packed with have been coated (1) (generator of centration of (1) of the generator sured by a modifi	l) in the effluent r column was mea- fication of the liquid chromato- that has been	<pre>(1) commercial product than 3% impurities (2) distilled over KMn and passed through packed with XAD-2 Hass, Philadelphia ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.002 mg(1)/kg (standard deviat REFERENCES: 1. May, W.; Chesler, S Gump, B.; Hertz, H. Dyszel, S. J. Chron 1975, 13, 535.</pre>	• O ₄ and NaOH a column (Rohm and , Pa). (2) ion) .; Cram, S.; ; Enagonio, D.;

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0]	May, W.E.; Wasik, S.P.; Freeman,
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	D.H. Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of fluoranthene in aqu	ueous sodium chloride is
reported in terms of the Setschenow e	equation:
$\log(S_{o}/S) = K_{S}C_{S}$	
where;	
S_ is the solubility of	of (1) in water (mg/L)
0	E (1) in saline solution (mg/L)
K _z is the Setschenow of	
5	
5	on of sodium chloride (mol/L)
evaluating the equation for S over the	ne range of C 0-0.7 mol/L,
$K_{\rm s} = 0.339$ with $S_{\rm o} = 0.206$.	
The corresponding mass percent and me	ole fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the com	pilers are $1.24 \text{ g} \times 10^{-5} \text{ g}(1)/100 \text{ g}$
sln and 1.14 x 10 ⁻⁸ .	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted	permanganate-sodium hydroxide
with an "extractor column" packed with a superficially porous bonded	and passed through an XAD-2 column.
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed	
through for extraction. The extract was introduced into a	
liquid chromatograph and the concen- tration of (1) was measured with a	ESTIMATED ERROR: temp ± 0.05°C
UV detector.	$K_{\pm} = 0.010$
	$s_0^s \pm 0.002$
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

Quantitative solubility data for pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in pyrene.

TABLE 1.	Quantitative	Solubility	Studies	of
	Pyrene (1)	in Water (2	<u>)</u>	

Reference	T/K	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Wauchope and Getzen (ref 3)	273-348	spectrophotometric
Mackay and Shiu (ref 4)	298	spectrofluorometric
Schwarz (ref 5)	285-304	spectrofluorometric
May et al. (ref 6)	298-302	chromatographic
Rossi and Thomas (ref 7)	298	GLC, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. At 298 K the values of Mackay and Shiu (ref 4), Schwarz (ref 5), May *et al.* (ref 6) and Rossi and Thomas (ref 7) are in excellent agreement and their average is Recommended. The values of Wauchope and Getzen (ref 3) and especially Klevens (ref 2) are signifigantly higher $(>3\sigma_n)$ than the other studies and are thus rejected. At 303 K the values of Wauchope and Getzen (ref 3) are in good agreement with those of Schwarz (ref 5) and May *et al.* (ref 6). At other temperatures the data are mainly those of Wauchope and Getzen and must therefore be regarded as Tentative.

With the exception of the rejected values noted above and the 300 K datum of Davis *et al.* (ref 1) which is omitted for representational convenience, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

COMPONENTS:	EVALUATOR:
<pre>(1) Pyrene; C₁₆H₁₀; [129-00-0] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

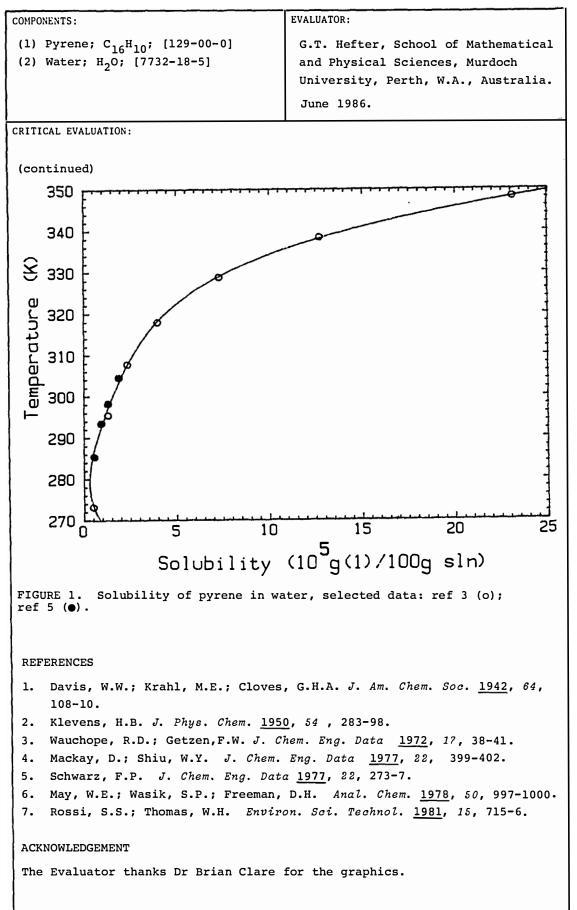
(continued)

TABLE 2. Recommended (R) and Tentative Solubility Values of Pyrene (1) in Water (2)

<i>т </i> к		ty values	L
	Reported values ^a	"Best" values (±ơ _r	
	10 ⁵ g(1)/100 g sln	10 ⁵ g(1)/100 g sln 1	10 ⁸ x ₁
273	0.49 (ref 3)	0.5	0.4
293	0.91* (ref 5)	0.9 0	0.8
298	1.35 (ref 4), 1.295 (ref 5),	1.32 ± 0.02(R)	.17(<i>R</i>)
	1.32 (ref 6), 1.3 (ref 7)		
303	1.80* (ref 3), 1.76* (ref 5),	1.75 ± 0.04(R)	L .56(R)
	1.70* (ref 6)		
313	3.30* (ref 3)	3 3	3
323	5.32 (ref 3)	5 4	1
333	9.4* (ref 3)	9 8	3
343	16.9 (ref 3)	17 15	5
348	23.1 (ref 3)	23 20)

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.



3	B_	3	7	4

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Pyrene; C₁₆H₁₀; [129-00-0] (2) Water; H₂0; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

Solubility of pyrene in water	
t/°C	10^4 g(1) L ⁻¹ (2)
27	1.60 ± 0,10
	1.65 ± 0.05

The best value recommended by the authors is 1.65×10^{-4} g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.65 x 10^{-5} g(1)/ 100 g sln and 1.45 x 10^{-8} .

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) prepared at Harvard University; m.p. range 149.6-150.5°C; (cf. ref 2). (2) dust-free. 	
	ESTIMATED ERROR: temp. ± 3°C	
	soly. see above	
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

The solubility of pyrene in water at 25°C was reported to be $1.75 \times 10^{-4} \text{ g(1)} \text{ L}^{-1} \text{ sln and } 7.7 \times 10^{-7} \text{ mol(1)} \text{ L}^{-1} \text{ sln.}$ Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.75 x $10^{-5} \text{ g(1)}/100 \text{ g sln and } 1.39 \times 10^{-8}$.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	(1) not specified.(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1972</u> , 17, 38-41.
VARIABLES:	PREPARED BY:
Temperature: 0-75°C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubility of pyrene in water	
$\frac{\text{mg(l)/kg(2)}}{\text{smoothed with}} = 10^5 \text{ g(l)/100 g sln} = 10^8 x_1$	

t/°C	experiment	smoothed with (std_dev)	10 ⁵ g(l)/100 g sln (compiler)	$10^8 x_1$ (compiler)
0.0 22.2 25.0 34.5 44.7 50.0 50.1 55.6 56.0 60.7 65.2 71.9	0.129, 0.128, 0.124 0.228, 0.235 0.397, 0.395, 0.405 0.558, 0.576, 0.556 0.75, 0.75, 0.77 0.74 0.96, 0.95, 0.90 1.27, 1.29 1.83, 1.86, 1.89	0.049(0.001) 0.130 0.148(0.002) 0.235 0.399 0.532(0.004) 0.534 0.73 0.74 0.97 1.27 1.90	0.49 1.30 1.48 2.35 3.99 5.32 5.34 7.3 7.4 9.7 12.7 19.0	0.44 1.15 1.32 2.09 3.55 4.74 4.75 6.5 6.6 8.6 11.3 16.9
74.7 75.0	2.21	2.26 2.31(0.03)	22.6 23.1	20.1 20.6

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Approximately 20 g of (1) was placed in each of three 250-mL glass- stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measure- ments. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by	 Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified. distilled and deionized. 	
	ESTIMATED ERROR:	
	temp. ± 0.5°C soly. see experimental values above	
serial dilution in calibrated glass- ware.	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Mackay, D.; Shiu, W.Y.	
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of pyrene in water at 25°C was reported to be 0.135 mg(1) dm ⁻³ sln and $x_1 = 1.2 \times 10^{-8}$. The corresponding mass percent calculated by the compiler		
is 0.0000135 g(l)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled.</pre>	
	ESTIMATED ERROR: soly. \pm 0.005 mg(1) dm ⁻³ sln (maximum deviation from several determinations).	
	REFERENCES :	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Water; H ₂ O; [7732-18-5]	Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 12.2-31.3°C	A. Maczynski

	Solubility of p	yrene in water	
t/°C	10 ⁷ mol(1) L ⁻¹	10 ⁶ g(1)/100 g sln (compiler)	$10^9 x_1$ (compiler)
12.2	2.70 ± 0.03	5.46	4.86
15.5	3.39 ± 0.03	6.86	6.11
17.4	3.91 ± 0.05	7.91	7.04
20.3	4.57 ± 0.04	9.25	8.23
23.0	5.78 ± 0.06	11.69	10.41
23.3	5.82 ± 0.03	11.77	10.48
25.0	6.40 ± 0.05	12.95	11.53
26.2	7.13 ± 0.07	14.42	12.84
26.7	7.18 ± 0.04	14.53	12.93
28.5	8.09 ± 0.08	16.37	16.90
31.3	9.3 ± 0.1	18.81	16.75

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Two methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells	 source not specified; better than 99 mole%, by glc; used as received. distilled over KMnO4 and NaOH and passed through a Sephadex column. 	
contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	ESTIMATED ERROR: temp. ± 0.1°C soly. see above REFERENCES:	

COMPONEN	TS:	ORIGINAL MEASUREMENTS:
(1) P3	rene; C ₁₆ H ₁₀ ; [129-00-0]	May, W.E.; Wasik, S.P.; Freeman, D.H.
(2) Wa	ater; H ₂ O; [7732-18-5]	Anal. Chem. <u>1978</u> , 50, 997-1000.
VARIABLE	S:	PREPARED BY:
Temper	cature: 25 and 29°C	A. Maczynski
EXPERIME	NTAL VALUES:	
	Solubility of p	-
t/°C	mg(l)/kg(2)	$\begin{array}{ccc} 10^5 \text{ g(l)/l00 g sln} & 10^8 x_1 \\ \underline{\qquad (compiler)} & (compiler) \end{array}$
25	0.132	1.32 1.18
29	0.162	1.62 1.44
1	411VT1 T 4 DV	INFORMATION
METHOD/A	PPARATUS /PROCEDURE:	
	• • • •	SOURCE AND PURITY OF MATERIALS:
	ynamic coupled column liquid atography (DCCLC) method was	(1) commercial product; less than 3% impurities.
based	on generating saturated solu- by pumping water through a	(2) distilled over KMnO ₄ and NaOH
column	n packed with glass beads that	and passed through a column
(1) (0	peen coated with the component generator column). The con-	packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).
	ation of (1) in the effluent e generator column was mea-	
sured	by a modification of the	
graphi	ed column liquid chromato- ic process that has been	ESTIMATED ERROR:
descr	ibed in ref 1.	temp. ± 0.05°C
		soly. ± 0.01 mg(1)/kg(2) (standard deviation)
		REFERENCES:
		<pre>1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.;</pre>
ļ		Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.
		<u>1775</u> , 10, 555.
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ORIGINAL MEASUREMENTS:
Rossi, S.S.; Thomas W.H. <i>Environ. Sci. Technol.</i> <u>1981</u> , <i>15</i> , 715-6.
PREPARED BY:
G.T. Hefter

The solubility of pyrene in distilled water at 25°C was reported to be 0.13 μ g/g, corresponding to a mole fraction, x_1 , of 6.4 x 10⁻¹⁰. The corresponding mass per cent calculated by the compiler is 1.3 x 10⁻⁵ g(1)/100 g sln.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
500 mL of water and an excess of (1) were equilibrated for at least 24 h in a 1 L Erlenmeyer flask placed in a constant temperature (±0.1°C) gyro- tary shaker (200 rpm). After a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a calibrated separatory funnel. Pyrene was isolated from solution by triplicate extraction with 10 mL of hexane (recovery >99%) and determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally determined by UV spectrophotometry (Beckman ACTA MVI). Agreement between GC and UV analyses was typically within 2%. Further details are given in the paper.	 (1) Aldrich; purified by derivati- zation with 2,4,6-trinitrophenol (2) Doubly distilled in all-glass apparatus; free of trace organics. ESTIMATED ERROR: Temperature: ±0.1°C Solubility: ±0.01 µg/g (std. dev. for 6 determinations)

COMPONENTS:	EVALUATOR:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

The solubility of pyrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Methods	Salinity g salts/kg sln	10 ⁶ g(1)100 g sln
Krasnoshchekova <i>et al</i> . (ref 1)	spectral	6	7.705
Schwarz (ref 2)	uv spectral	30	9.48
May et al. (ref 3)	HPLC	35	8.60
Rossi and Thomas (ref 4)	GLC	35	8.9

At 298 K and a salinity of 35 g salts/kg sln the data of May $et \ al$. and Rossi and Thomas are in very good agreement. Since the value reported by May $et \ al$. is more precise and derived from several measurements using the Setschenow equation, it is adopted as the recommended value for the solubility of pyrene in seawater at the temperature and salinity indicated. Rossi and Thomas and Schwarz each report data over a range of temperatures.

 $\frac{\text{SOLUBILITY OF PYRENE (1) IN SEAWATER (2)}}{\frac{\text{RECOMMENDED VALUE}}{298}} \frac{10^6 \text{ g(1)/100 g sln}}{35}$

REFERENCES

- Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.
- 2. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 3. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.
- 4. Rossi, S.S.; Thomas, W.H. Environ. Sci. Technol. <u>1981</u>, 15, 715-6.

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of pyrene in salt wat to be 78.9 μ g/L.	
The corresponding mass percent and m by the compilers are 7.705 x 10 ⁻⁶ g(assuming a solution density of 1.004	$1)/100 \text{ g sln and } 7.02 \times 10^{-9}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen-	
trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis	ESTIMATED ERROR: temp. ± 1°C soly. ± 2.93 type of error not specified
of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	REFERENCES: 1. Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya <u>1973</u> , 13, 885.

CONDONENTS			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [3		Schwarz, F.P.	
(2) Sodium chloride; 1 [7647-14-5]	NaCl;	J. Chem. Eng. Data <u>1977</u> , 22, 273-7.	
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES:	140	PREPARED BY:	
Temperature: 8.6-31.		W.Y. Shiu, D. Mackay	
Salinity: 30 g(2)/kg	sln		
EXPERIMENTAL VALUES:			
Solu	bility of pyrene	in 0.5 g-mol(2)/dm ³	
<u>t.</u>	/°C	10 ⁷ mol(1)/L sln	
	8.6	, 2.00	
	2.2	2.50	
	5.5	2.85	
	8.2 0.7	3.22 3.57	
	3.0	3.90	
•	5.0	4.41	
	8.1	5.19	
3.	1.1	5.96	
7.97×10^{-9} .			1
7.97 x 10 ⁻ .			
7.97 x 10 ⁻ .	AUXILIARY	INFORMATION	
7.97 x 10 ⁻ . METHOD/APPARATUS/PROCEDURE:		,	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr	: ene in NaCl so-	INFORMATION	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined	ene in NaCl so-	SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %,	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr	ene in NaCl so- by fluore- ion measure-	SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa	ene in NaCl so- by fluore- ion measure- scence method, s prepared by	SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %,	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount	: by fluore- ion measure- scence method, s prepared by of pyrene to	SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade,	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount of an air-tight 1 x 1 cm	: by fluore- ion measure- scence method, s prepared by of pyrene to quartz fluore-	SOURCE AND FURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO4 -	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount	: by fluore- cion measure- escence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt	SOURCE AND FURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containin; solution. The cell w 20 rpm for at least 7	: by fluore- tion measure- escence method, s prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther-	SOURCE AND FURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO4 -	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath a	: rene in NaCl so- by fluore- sion measure- escence method, s prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther- nd then its	SOURCE AND FURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath a: fluorescent intensity	: tene in NaCl so- by fluore- ion measure- scence method, s prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured	SOURCE AND FURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath a: fluorescent intensity	: rene in NaCl so- by fluore- ion measure- scence method, s prepared by of pyrene to a quartz fluore- g 5 mL salt ras rotated at 2 hr in a ther- nd then its was measured profluorimeter	SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex colum	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath at fluorescent intensity at 395 nm. The Spect employed a ratio-photo mode where pyrene con	: Tene in NaCl so- by fluore- ion measure- scence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting centration was	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum ESTIMATED ERROR: Solubility ± 1.6% (author)</pre>	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath as fluorescent intensity at 395 nm. The Spect employed a ratio-photo mode where pyrene con linearly related to t	: rene in NaCl so- by fluore- ion measure- scence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence	SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex colum	1
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount of an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath at fluorescent intensity at 395 nm. The Spect employed a ratio-photo mode where pyrene con linearly related to tt signal. The UV metho	: rene in NaCl so- by fluore- ion measure- escence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther- nd then its was measured trofluorimeter on counting icentration was he fluorescence d was used to	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum ESTIMATED ERROR: Solubility ± 1.6% (author)</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath as fluorescent intensity at 395 nm. The Spect employed a ratio-photo mode where pyrene con linearly related to t	: rene in NaCl so- by fluore- ion measure- escence method, s prepared by of pyrene to a quartz fluore- g 5 mL salt as rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting centration was he fluorescence d was used to ty of pyrene	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath ai fluorescent intensity at 395 nm. The Spect: employed a ratio-photo mode where pyrene con linearly related to t signal. The UV metho obtain the absorptivi in ethanol therefore absolute solubility s	: rene in NaCl so- by fluore- ion measure- iscence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence d was used to ty of pyrene provide an	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath at fluorescent intensity at 395 nm. The Spect employed a ratio-photo mode where pyrene con linearly related to t signal. The UV methoo obtain the absorptivi in ethanol therefore	: rene in NaCl so- by fluore- ion measure- iscence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence d was used to ty of pyrene provide an	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath ai fluorescent intensity at 395 nm. The Spect: employed a ratio-photo mode where pyrene con linearly related to t signal. The UV metho obtain the absorptivi in ethanol therefore absolute solubility s	: rene in NaCl so- by fluore- ion measure- iscence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence d was used to ty of pyrene provide an	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath ai fluorescent intensity at 395 nm. The Spect: employed a ratio-photo mode where pyrene con linearly related to t signal. The UV metho obtain the absorptivi in ethanol therefore absolute solubility s	: rene in NaCl so- by fluore- ion measure- iscence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence d was used to ty of pyrene provide an	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	
METHOD/APPARATUS/PROCEDURE: The solubility of pyr lution was determined scence and UV absorpt ments. In the fluore saturated solution wa adding excess amount an air-tight 1 x 1 cm scence cell containing solution. The cell w 20 rpm for at least 7 mostated water bath ai fluorescent intensity at 395 nm. The Spect: employed a ratio-photo mode where pyrene con linearly related to t signal. The UV metho obtain the absorptivi in ethanol therefore absolute solubility s	: rene in NaCl so- by fluore- ion measure- iscence method, is prepared by of pyrene to a quartz fluore- g 5 mL salt vas rotated at 2 hr in a ther- nd then its was measured rofluorimeter on counting icentration was he fluorescence d was used to ty of pyrene provide an	<pre>SOURCE AND PURITY OF MATERIALS: Pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO₄ - NaOH solution and passed through a Sephadex colum</pre>	

	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]	May, W.E.; Wasik, S.P.; Freeman, D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	
The solubility of pyrene in aqueous	sodium chloride is
reported in terms of the Setschenow	equation:
$\log(S_{o}/S) = K_{s}C_{s}$	
where;	
S _o is the solubility	of (1) in water (mg/L)
S is the solubility of	E (1) in saline solution (mg/L)
K _s is the Setschenow	constant (L/mol)
C in the concentration	on of sodium chloride (mol/L)
evaluating the equation for S over the	
$K_{\rm g} = 0.286$ with $S_{\rm O} = 0.132$.	- S
s s s o s o	
The corresponding mass percent and m	ole fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the compilers are 8.60 x 10^{-6} g(1)/100 g sln	
and 7.84 x 10^{-9} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was	(1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted	permanganate-sodium hydroxide
with an "extractor column" packed with a superficially porous bonded	and passed through an XAD-2 column.
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed	
through for extraction. The	
extract was introduced into a liquid chromatograph and the concen-	ESTIMATED ERROR:
tration of (1) was measured with a UV detector.	temp ± 0.05°C
	K _s ± 0.003 S _o ± 0.001
	REFERENCES:

OMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0]		Rossi, S.S.; Thomas, W.H.	
(2) Seawater; natural		Environ. Sci. Technol. <u>1981</u> , 15, 715-6.	
VARIABLES: PREPARED BY:			
25°C	W.Y. Shiu,	W Y Shin D Mackay	
sln			
	•		
Solubility o	of pyrene in seaw	ater	
µg(l)/g(2)	l0 ⁶ Mass% ^a g(l)/l00 g sln	10 ⁹ ^x 1 ^a	
0.056 0.071 0.089	5.6 7.1 8.9	5.1 6.5 8.1	
AUXII	LIARY INFORMATION		
ater with an or at least 2 erature gyrota a 12 hr sta- ion period. A extracted the e. The concer act was analy raph equipped detector to	by Pyrene: 4 hr. ary n-Hexane: A ree Seawater: Pier and 0.22 µm m tracted w salinity ion. ESTIMATED ERRO	<pre>from Aldrich Chemi and purified with 2,4,6-trinitropher doubly distilled glass. collected off So was filtered twice embrane and twice ith n-hexane then was adjusted to 35 R: y ± 11%</pre>	nol. d in cripps e through ex- its
	AUXII RE: was prepared ated by compil AUXII RE: was prepared ater with an or at least 2- erature gyrota a 12 hr sta- ion period. A extracted the extracted the concernent of the extracted the ater with an analy ater with analy a stracted the extracted the extracted the ater with analy a stracted the extracted the ater with analy a stracted the ater was analy ater with analy ater with analy ater was analy ater with analy ater with analy ater was analy ater with analy ater	x [129-00-0] Rossi, S.S. x [120-00-0] Rossi, S.S. x [100-0] Soluze x [100-0] Rossi, S.S. x [100-0] Rossi, S.S. x [100-0] Rossi, S.S. x [100-0] Rossi, S.S. x [100-0] Soluze	x: [129-00-0] Rossi, S.S.; Thomas, W.H. rcal Environ. Sci. Technol. 198; 715-6. 25°C W.Y. Shiu, D. Mackay solubility of pyrene in seawater ug(1)/g(2) 10 ⁶ Mass% ^a 10 ⁹ x ₁ ^a

38_386	461
COMPONENTS:	ORIGINAL MEASUREMENTS:
 9,10-Dimethylanthracene; 	Mackay, D.; Shiu, W.Y.
C ₁₆ H ₁₄ ; [781-43-1]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 9,10-dimethylanthra to be 0.056 mg(1) dm ⁻³ sln and $x_1 = 4$ The corresponding mass percent calcul is 5.6 x 10 ⁻⁶ g(1)/100 g sln.	$.90 \times 10^{-9}$.
AUXILIARY	INFORMATION
METHOD /APPARATUS /PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs.	 Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. doubly distilled.
the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. \pm 0.0005 mg(1) dm ⁻³ sln
	(maximum deviation from several

ESTIMATED ERROR:

soly. ± 0.0005 mg(1) dm⁻³ sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trimethyl-2-phenylheptene; C ₁₆ H ₂₆ ; [4810-06-4]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 10-30°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of Water in 2,4,6	5-Trimethy1-2-phenylheptene
$t/^{\circ}C$ g(2)/100 g slr	$10^3 x_2$ (compiler)
10 0.0096 20 0.0154 30 0.0252	1.16 1.87 3.05
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving	(1) Not specified.(2) Not specified.
hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	
	ESTIMATED ERROR:
	ESTIMATED ERROR: Not specified.
	Not specified.
	Not specified.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 7,8-Dimethyltetradecane; C₁₆H₃₄; [2801-86-7]</pre>	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H ₂ O; [7732-18-5]	Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-50°C	A. Maczynski and M.C. Haulait-Pirson

Solubility of w	vater in 7,8-dimethylt	etradecane
<i>t</i> /°C	g(2)/100 g sln	10 ⁴ x ₂ (compiler)
20	0.0077	9.67
30	0.0134	16.83
40	0.0219	27.48
50	0.0344	43.09

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Component (1) was introduced into a thermostatted flask and saturated for	(1) not specified.	
5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(2) not specified.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS:	EVALUATOR:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

TABLE 1.

Quantitative solubility data for the hexadecane (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Englin et al. (ref 2)	293-323	(2) in (1)	analytical
Franks (ref 3)	298	(1) in (2)	GLC
Yoshida and Yamane (ref 4)	_ <i>a</i>	(1) in (2)	GLC
Skripka and Namiot (ref 5)	598 ^b	(2) in (1)	_ ^a
Sutton and Calder (ref 6)	298	(1) in (2)	GLC
Skripka and Sultanov (ref 7,8)	523-598 ^b	(2) in (1)	_a

Hexadecane (1) - Water (2) System

Quantitative Solubility Studies of the

a Not specified.

b Pressure also varied.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF HEXADECANE (1) IN WATER (2)

All data on the solubility of hexadecane in water have probably been obtained at 298 K (Table 1, although Yoshida and Yamane (ref 4) did not specify their temperature). However the values are in poor agreement and no "best" value has been calculated. It may also be noted that all values are higher than the value of $\sim 2 \times 10^{-9}$ g(1)/100 g sln predicted by extrapolation of lower hydrocarbon solubilities (although whether this extrapolation remains valid for very long chain hydrocarbons is not known).

T/K	Reported values ^a
	10 ⁷ g(1)/100 g sln
298	6.3 (ref 3), 5.57 ^b (ref 4), 0.9 (ref 6)

COMPONENTS:	EVALUATOR:
<pre>(1) Hexadecane; C₁₆H₃₄; [544-76-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

(continued)

2. THE SOLUBILITY OF WATER (2) IN HEXADECANE (1)

The solubility of water in hexadecane at atmospheric pressure have been reported by Schatzberg (ref 1) and Englin *et al.* (ref 2) over a range of temperatures. However, agreement is poor (Table 3) and the data must be considered as very Tentative.

TABLE 3. Tentative Solubility Values ofWater (2) in Hexadecane (1)

T/K	Solubility values		
	Reported values 10 ³ g(2)/100 g sln	"Best" values 10 ³ g(2)/100 g sln	
293	6.9 (ref 2)	7	0.9
298	5.4 (ref 1), 9.6 ^a (ref 2)	8 ± 2	1.0
303	12.3 (ref 2)	12	1.5
313	10.4 (ref 1), 20.9 (ref 2)	16 ± 5	2.0
323	33.2	33	4.2

a Obtained by the Evaluator by graphical interpolation of the authors' data.

b Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

At higher pressures the solubility of water in hexadecane has been reported over the range 523-598 K and 1.7-78.5 MPa by Skripka *et al.* (ref 5, 7, 8). As these are the only data available under these conditions no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

- 1. Schatzberg, P. J. Phys. Chem. 1963, 67, 776-9.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u>, 10, 42-6.
- 3. Franks, F. Nature (London) 1966, 210, 87-8.
- 4. Yoshida, F.; Yamane, T. Biotechnol. Bioenerg. <u>1971</u>, 13, 691-6.
- 5. Skripka, V.G.; Namiot, A.Yu. Zh. Fiz. Khim. <u>1974</u>, 48, 782.
- 6. Sutton, C.; Calder, J.A. Environ. Sci. Technol. 1974, 8, 654-7.
- 7. Skripka, V.G.; Tr. Vses. Neftegazov Nauch Issled. Inst. 1976, 61, 139-51.
- 8. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. <u>1973</u>, 47, 1035.

400	50_590
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Schatzberg, P.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1963</u> , 67, 776-9.
VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of water	in hexadecane
t/°C mg(2)/	kg sln <u>x2</u>
25 54	a 6.8×10^{-4}
40 104	
a,b See "Estimated Error"	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and com- pletely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro- phobized hypodermic syringe. Sta- bilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Humphrey-Wilkinson, Inc.; ASIM normal cetane; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range. (2) distilled and deionized. (2) distilled and deionized. ESTIMATED ERROR: temp. ± 0.02°C soly. a) 0-6%; b) 0-2% (deviations from the mean) REFERENCES:</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. Khim. Tekhnol. Topl. Masel <u>1965</u> , 10, 42-6.
VARIABLES:	PREPARED BY:
Temperature: 20-50°C	A. Maczynski and M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of wat	er in hexadecane
t/°C g(2)/	100 g sln $10^4 x_2$
	(compiler)

		<u>(compilér)</u>
20	0.0069	8.67
30	0.0123	15.45
40	0.0209	26.22
50	0.0332	41.59

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) not specified.(2) not specified.		
	ESTIMATED ERROR:		
	not specified.		
	REFERENCES:		

468	38_392
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3] (2) Water; H ₂ O; [7732-18-5]	Franks, F. Nature (London) <u>1966</u> , 210, 87-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
The solubility of hexadecane in water in mole fraction $x_1 = 5 \times 10^{-10}$. The corresponding mass percent calcul 6.3 $\times 10^{-7}$ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chroma- tographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka; purum grade; purity > 97% (chromatographic analysis). (2) not specified. ESTIMATED ERROR:</pre>

soly. ± 12%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Yoshida, F.; Yamane, T.
(2) Water, H ₂ O; [7732-18-5]	Biotechnol. Bioeng. <u>1971</u> , 13, 691-6.
VARIABLES:	PREPARED BY:
One temperature: not specified	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of hexadecane in water g(l) cm ⁻³ sln.	was reported to be 5.57 x 10^{-9}
With the assumption that a solution d ponding mass percent and mole fractio are 5.57 x 10^{-7} g(1)/100 g sln and 4.	on, x_1 , calculated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. 10 mL of (1) and 1200 mL of (2) were placed in a stoppered flask and agitated with a magnetic stirrer	not specified.
at a speed of 200 rpm for 9 to 24 hrs. (1) was extracted from 1000 ml of (2) with 2 mL of heptane and its concentration determined by gas chromatography using a Shimadzu	
equipped with hydrogen flame de- tectors.	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]		Skripka, V.G.;	Namiot, A.Yu.	
(2) Water; H ₂ O; [7732-18-5] VARIABLES:		Zh. Fiz. Khim.	<u>1974</u> , <i>48</i> , 782.	
		PREPARED BY:		
One temperature: 325 Pressure: 1.7-13.18 M	°C MPa	A. Maczynski		
EXPERIMENTAL VALUES:				
	lity of water in	hexadecane at 32	5°C	
p/kg cm ⁻²	p/MPa (compiler)	<i>x</i> 2	g(2)/100 g sln (compiler)	
17.3	1.7	0.083	0.71	
41.5	4.07	0.232	2.34	
62.5	6.13	0.352	4.14	
94.2	9.24	0.517	7.85	
134.4	13.18	0.712	16.43	
	AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE		INFORMATION SOURCE AND PURITY O	F MATERIALS:	
METHOD/APPARATUS/PROCEDURE Method was described Nothing more was repo paper.	in refs 1 and 2	SOURCE AND PURITY O		
Method was described Nothing more was repo	in refs 1 and 2	SOURCE AND PURITY O	specified; CP	
Method was described Nothing more was repo	in refs 1 and 2	SOURCE AND PURITY O (1) source not reagent; us	specified; CP	
Method was described Nothing more was repo	in refs 1 and 2	SOURCE AND PURITY O (1) source not reagent; us	specified; CP	
Method was described Nothing more was repo	in refs 1 and 2	SOURCE AND PURITY O (1) source not reagent; us (2) distilled.	specified; CP	
Method was described Nothing more was repo	in refs 1 and 2	SOURCE AND PURITY O (1) source not reagent; us (2) distilled. ESTIMATED ERROR: not specified. REFERENCES: 1. Sultanov, R. Namiot, A.Yu 2, 57.	specified; CP	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ [544-	76-3] Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

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The solubility of hexadecane in water at 25°C was reported to be 0.9 x 10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 0.7 x 10^{-10}.
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AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:

				50_590
COMPONENTS :			ORIGINAL MEASUREMENTS	3:
	ecane; C ₁₆ H ₃₄ ; [; H ₂ 0; [7732-18-		Skripka, V.G. Tr. Vses. Nefteg Inst. <u>1976</u> , 6 Sultanov, R.G.; Zh. Fiz. Khim.	Skripka, V.G.
ARIABLES:			PREPARED BY:	
Temperatu: Pressure:	re: 250-325°C 3.9-78.5 MPa		A. Maczynski	
EXPERIMENTAL	VALUES: Solubil	ity of wate	r in hexadecane	
t/°C	$p/kg cm^{-2}$	p/MPa (compil	er) ^x 2	g(2)/100 g sln (compiler)
250 275	40 53 93 100 134 150 200 300 400 500 600 700 800 53 93 100 134 150 200 300 400 500 600 700 800	3.9 5.2 9.1 9.8 13.1 14.7 19.6 29.4 39.0 58.8 68.6 78.5 5.2 9.1 9.8 13.1 14.7 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.227 0.217 0.216 0.212 0.211 0.208 0.197 0.193 0.190 0.186 0.182 0.178 0.355 0.345 0.343 0.336 0.333 0.325 0.308 0.290	2.32 2.28 2.16 2.14 2.00 2.08 2.05 1.91 1.87 1.83 1.78 1.74 1.69 4.19 4.02 3.99 3.87 3.82 3.69 3.42 3.15 2.90 2.72 2.58 2.50 (continued)
		AUXILIARY	INFORMATION	
		UNITIUNI		
The exper described	ATUS/PROCEDURE: imental techniqu in ref l. No d in the paper.		reagent grad	MATERIALS: specified, chemical le; purity not used as received.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. <u>1971</u>, 4, 6.

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	ecane; C ₁₆ H ₃₄ ; [544- ; H ₂ 0; [7732-18-5]	Tr. Vs.		gazov. Nauch. Issled. 1, 139-51.
	-	Sultano Zh. Fi:	ov, R.G.; z. Khim.]	Skripka, V.G. 1973, 47, 1035.
t/°C	p/kg cm ⁻²	p/MPa	<i>*</i> 2	g(2)/100 g sln

		(compiler)		(compiler)
300	93	9.1	0.517	7.84
	100	9.8	0.505	7.51
	134	13.1	0.480	6.84
	150	14.7	0.469	6.56
	200	19.6	0.441	5.90
	300	29.4	0.404	5.11
	400	39.2	0.384	4.72
	500	49.0	0.366	4.39
	600	58.8	0.348	4.07
	700	68.6	0.329	3.75
	800	78.5	0.310	3.45
325	134	13.1	0.712	16.43
	150	14.7	0.643	12.53
	200	19.6	0.571	9.57
	300	29.4	0.509	7.62
	400	39.2	0.480	6.84
	500	49.0	0.466	6.49
	600	58.8	0.450	6.11
	700	68.6	0.435	5.77
	800	78.5	0.414	5.32

174	38_397
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Hexadecane; C ₁₆ H ₃₄ ; [544-76-3]	Sutton, C.; Calder, J.A.
(2) Seawater	Environ. Sci. Technol. <u>1974</u> ,
	8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of hexadecane in seawa 4 x 10^{-8} g(1)/100 g sln and $x_1 = 3$ x	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
(1) and (2) were placed in a glass	SOURCE AND PURITY OF MATERIALS: Analabs, Inc., North Haven, Conn.
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at 25.0 \pm 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<pre>99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre>
	made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of

natural dissolved organic matter. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]fluorene; C ₁₇ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[238-84-3]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
2	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of Benzo[a]fluorene to be 0.045 mg(l) dm ⁻³ sln and $x_1 = 1$	
The corresponding mass percent calculis 4.5×10^{-6} g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	(2) doubly distilled.
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. ± 0.0012 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

COMPONENTS: (1) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H ₂ O; [7732-18-5]	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.
	June 1986.

Quantitative solubility data for benz[a]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in bena[a]anthracene.

TABLE 1.	Quantitative	Solubility	Studies	of
Benz	[a] anthracene	(1) in Wate	er (2)	

Reference	T/K	Method
Davis et al. (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In general the available data are in good agreement given the very low solubility of benz[a]anthracene in water. Although the data of Mackay and Shiu is somewhat higher than all other values there are at the present time insufficient grounds for its rejection. The available data are summarized in Table 2 and may be regarded as Tentative.

	Tentative S					of
Benz[a] anthracene	(1)	in V	Vater	(2)	

<i>т</i> /к	Solubilit	y values	
	Reported values	"Best" values	
	10 ⁶ g(1)/100 g sln	10 ⁶ g(1)/100 g sln	10 ¹⁰ x ₁
298	0.983 (ref 2), 1.4 (ref 3), 0.94 (ref 4)	1.1 ± 0.2	9
300	1.1 (ref 1)	1.1	9
302	1.22 (ref 4)	1.2	9

a Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

COMPONENTS: (1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3] (2) Water; H₂O; [7732-18-5] EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

(continued)

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

38	4	01

38_401	47
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Benz[a]anthracene; C₁₈^H₁₂; [56-55-3]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of benz[a]ant	chracene in water
t/°C	10 ⁵ g(1) L ⁻¹ (2)
27	1.1
	1.1
	1.2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	 (1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2). (2) dust-free.
Many details are reported in ref 1.	ESTIMATED ERROR: temp. $\pm 3^{\circ}$ C soly. $\pm 0.1 \times 10^{-5}$ g(1) dm ⁻³ (2)

480	38_402
COMPONENTS: (1) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Klevens, H.B. J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
Temperature: 25°CM.C. Haulait-PirsonEXPERIMENTAL VALUES:The solubility of benz[a]anthracene in water at 25°C was reported to be 10^{-5} g(1) L ⁻¹ sln and 4.31 x 10^{-8} mol(1) L ⁻¹ sln.Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 9.83 x 10^{-7} g(1)/ 100 g sln and 7.78 x 10^{-10} .	

SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
ESTIMATED ERROR:
not specified.
REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; C ₁₈ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[56-55-3]	J. Chem. Eng. Data <u>1977</u> , 22,
(2) Water; H ₂ O; [7732-18-5]	399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of benz[a]anthracene to be 0.014 mg(1) dm ⁻³ sln and $x_1 = 1$ The corresponding mass percent calcul is 1.4 x 10 ⁻⁶ g(1)/100 g sln.	$.1 \times 10^{-9}$.
AUXILIARY	INFORMATION
METHOD /AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for	 Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. doubly distilled.
analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. \pm 0.0002 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) Benz[a]anthracene; C₁₈H₁₂; [56-55-3] (2) Water; H₂O; [7732-18-5]</pre>	May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u> , 50, 997-1000.			
VARIABLES:	PREPARED BY:			
Temperature: 25 and 29°C	A. Maczynski			
EXPERIMENTAL VALUES:				
Solubility of benz[a]anthracene in water				
t/°C mg(1)/kg(2)	$\frac{10^6 \text{ g(l)/100 g sln}}{(\text{compiler})} \qquad \frac{10^{10} x_1}{(\text{compiler})}$			
25 0.0094	0.94 7.4			
29 0.0122	1.22 9.6			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concen- tration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic pro- cess that has been described in ref 1.	<pre>(1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Haas, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2) (stand. dev.) REFERENCES: 1. May, W.; Chesler, S.; Cram, S.; Gump, B; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.</pre>			

COMPONENTS:	EVALUATOR:
 (1) Benz[a]anthracene; C₁₈H₁₂; [55-56-3] (2) Seawater 	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982
CRITICAL EVALUATION:	

The solubility of benz[a]anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln 	10 ⁷ g(l)/100 g sln
Krasnoshchekova <i>et al</i> . (ref 1)	spectral	6	0.62
May et al. (ref 2)	HPLC	35	5.6

The value reported by May *et al*. was derived from several measurements using the Setschenow equation and is consistent with the recommended value for the solubility of benz[a]anthracene in pure water. Therefore their value is adopted as tentative. The value of Krasnoshchekova *et al*. appears slightly low and is considered doubtful.

> SOLUBILITY OF BENZ[A]ANTHRACENE (1) IN SEAWATER (2) TENTATIVE VALUE

T/K	g salts/kg sln	10 ⁷ g(1)/100 g sln
298	35	5.6

REFERENCES

- Krasnoshchekova, R.Ya.; Pakpill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.
- May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

m	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11(2), 133-6.
VARIABLES :	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of benz[a] anthracene to be 0.63 μ g/L.	in salt water was reported
The corresponding mass percent and mo by the compilers are 6.2 x 10^{-8} g(1)/ assuming a solution density of 1.004	$100 \text{ g sln and } 5.2 \times 10^{-11}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	Not given.

COMPONENTS: (1) Benz[a]anthracene; C ₁₈ H ₁₂ ; [56-55-3]	ORIGINAL MEASUREMENTS: May, W.E.; Wasik, S.P.; Freeman, D.H.
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES: One temperature: 25°C	PREPARED BY:
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES:	I
The solubility of benz[a]anthracene i	n aqueous sodium chloride is
reported in terms of the Setschenow e	quation:
$\log(S_{o}/S) = K_{s}C_{s}$	
where;	
S_{o} is the solubility of	f (1) in water (mg/L)
S is the solubility of	(1) in saline solution (mg/L)
K _s is the Setschenow c	onstant (L/mol)
C _s in the concentratio	n of sodium chloride (mol/L)
evaluating the equation for S over th	e range of C _s 0-0.7 mol/L,
$K_{\rm S} = 0.354$ with $S_{\rm O} = 0.0094$.	
The corresponding mass percent and mo	le fraction x_1 , at salinity =
35 g(2)/kg sln calculated by the comp	ilers are 5.6 x 10 ⁻⁷ g(1)/100 g
sln and 4.5×10^{-10} .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) was	SOURCE AND PURITY OF MATERIALS: (1) greater than 97% pure.
prepared by pumping salt water through a "generation column" which	(2) reagent grade.
was packed with glass beads coated with 1% by weight of (1). The	(3) distilled from potassium
saturated solution was extracted with an "extractor column" packed	permanganate-sodium hydroxide and passed through an XAD-2
with a superficially porous bonded	column.
C ₁₈ stationary phase, then a water- acetonitrile solvent was passed	
through for extraction. The extract was introduced into a	
liquid chromatograph and the concen- tration of (1) was measured with a	ESTIMATED ERROR:
UV detector.	temp ± 0.05°C K _s ± 0.002
	s ± 0.001
	REFERENCES :

38_408

COMPONENTS:	EVALUATOR:
<pre>(1) Chrysene; C₁₈H₁₂; [218-01-9] (2) Water; H₂0; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.
	June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for chrysene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in chrysene.

TABLE 1.	Quantitative Solubil: Chrysene (1) in Water	
Reference	<i>Т/</i> К	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May et al. (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of Klevens (ref 2) value at 298K, which is very much higher than other studies (ref 3,4) and is therefore rejected, all the available data are summarized in Table 2 below. The solubilities are in reasonable agreement although their limited number and temperature range suggests a Tentative classification at this stage.

TABLE						Values	for
	C	nrysene	(1)	in	Water	(2)	

<i>т</i> /к	Solubil	ity values	
	Reported values	"Best" values	$(\pm \sigma_n)^a$
	10 ⁷ g(1)/100 g sln	10 ⁷ g(1)/100 g sln	10 ¹⁰ <i>x</i> 1
298	2.0 (ref 3), 1.8 (ref 4)	1.9 ± 0.1	1.5
300 302	1.5 (ref 1)	1.5	1.2
302	2.2 (ref 4)	2.2	1.7

a Obtained by averaging where appropriate; σ_{n} has no statistical significance.

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(continued next page)

COMPONENTS :	EVALUATOR:
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.
	June 1986.
CRITICAL EVALUATION: (continued)	
REFERENCES	
 Davis, W.W.; Krahl, M.E.; Clove 108-10. 	s, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64,
2. Klevens, H.B. J. Phys. Chem.	<u>1950, 54, 283.</u>
2 Nochow D. Chiw M.V. J. Chaw	

- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.
- 4. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u>, 50, 997-1000.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Chrysene; C₁₈H₁₂; [218-01-9] (2) Water; H₂O; [7732-18-5]</pre>	<pre>Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.</pre>
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility	of chrysene in water
t/°C	10^{6} g(1) L ⁻¹ (2)
27	1.5 ± 0.5
	1.5 ± 0.2

The best value recommended by the authors is 1.5×10^{-6} g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.5 x 10^{-7} g(1)/ 100 g sln and 1.2 x 10^{-10} .

AUXILIARY INFORMATION

1	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 prepared at Harvard University; m.p. range 253.2-253.8°C; (cf. ref 2). dust-free.
	ESTIMATED ERROR:
	temp. ± 3°C soly. see above
	REFERENCES:
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc <u>1942</u>, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of chrysene in water a	t 25°C was reported to be

The solubility of chrysene in water at 25 c was reported to be $6 \times 10^{-6} \text{ g(1) } \text{L}^{-1} \text{ sln and } 2.76 \times 10^{-8} \text{ mol(1) } \text{L}^{-1} \text{ sln.}$ Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 6.29 x $10^{-7} \text{ g(1)}/$ 100 g sln and 4.98 x 10^{-10} .

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.		
	ESTIMATED ERROR: not specified. REFERENCES:		

ORIGINAL MEASUREMENTS:
Mackay, D.; Shiu, W.Y.
J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
PREPARED BY:
M.C. Haulait-Pirson
at 25°C was reported 1.58 x 10 ⁻¹⁰ . lated by the compiler
INFORMATION
<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.00017 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES: </pre>

10 12 Anal. Chem. 1978, 50, 997-1000. (2) Water; H ₂ O; [7732-18-5] Anal. Chem. 1978, 50, 997-1000. VARIABLES: Temperature: 25 and 29°C Solubility of chrysene in water t/°C O.0018 1.8 25 0.0018 1.8 AUXILIARY INFORMATION MUNILIARY INFORMATION	38_412	491
10 12 Anal. Chem. 1978, 50, 997-1000. VARIABLES: Temperature: 25 and 29°C Solubility of chrysene in water t/°C Solubility of chrysene in water 10 ⁷ g(1)/100 g sln (compiler) (compiler) (compiler) 2.2 AUXILIARY INFORMATION MUNIMARY INFORMATION	COMPONENTS:	ORIGINAL MEASUREMENTS:
A. Maczynski EXPERIMENTAL VALUES: Solubility of chrysene in water t/°C mg(1)/kg(2) 10 ⁷ g(1)/100 g sln (compiler) 25 0.0018 1.8 1.4 29 0.0022 2.2 1.7 MUNILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. Source AND PURITY OF MATENIALS: ESTIMATED ERNOR: ESTIMATED ERNOR: temp. ± 0.05°C soly. to 0.001 mg(1)/kg(2) (standard deviation)	10 12	May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. <u>1978</u> , 50, 997-1000.
A. Maczynski EXPERIMENTAL VALUES: Solubility of chrysene in water t/*C mg(1)/kg(2) 10 ⁷ g(1)/100 g sln (compiler) 10 ¹⁰ x1 (compiler) 25 0.0018 1.8 1.4 29 0.0022 2.2 1.7 MUNITARY INFORMATION METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. Source AND PURITY OF MATENIALS: ESTIMATED ERNOR: ESTIMATED ERNOR: temp. ± 0.05°C soly. to 0.001 mg(1)/kg(2) (standard deviation)	VARIABLES:	PREPARED BY:
Solubility of chrysene in water t/*C mg(1)/kg(2) 10 ⁷ g(1)/100 g sln (compiler) 10 ¹⁰ x1 (compiler) 25 0.0018 1.8 1.4 29 0.0022 2.2 1.7 AUXILIARY INFORMATION METHOD/AFPARTUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. SOURCE AND PURITY OF MATERIALS: STIMATED ERRON: (2) distilled over KMnO, and NaOH and passed through a column backed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. ESTIMATED ERRON: ESTIMATED ERRON: Cols ⁵ C (standard deviation)		
t/*C mg(1)/kg(2) 10 ⁷ g(1)/100 g sln (compiler) 10 ¹⁰ x1 (compiler) 25 0.0018 1.8 1.4 29 0.0022 2.2 1.7 MULLIARY INFORMATION SURCE AND PURITY OF MATERIALS: <tr< td=""><td>EXPERIMENTAL VALUES:</td><td></td></tr<>	EXPERIMENTAL VALUES:	
t/°C mg(1)/kg(2) 10 ⁷ g(1)/100 g sln (compiler) 10 ¹⁰ x1 (compiler) 25 0.0018 1.8 1.4 29 0.0022 2.2 1.7 AUXILIARY INFORMATION METHOD/AFPARATUS/FROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. SURCE AND PURITY OF MATERIALS: ESTIMATED ERROR: ESTIMATED ERROR: ESTIMATED ERROR: ESTIMATED ERROR:	Solubility of chr	ysene in water
29 0.0022 2.2 1.7 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The contration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatography (Decce) that has been described in ref 1. Source AND FURITY OF MATERIALS: Source ERROR: Estimated ERROR:	-	$10^7 q(1)/100 q sln = 10^{10} x_1$
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been described in ref 1. SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. ESTIMATED ERROR: (2) distilled over KMnO4, and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2) (standard deviation)	25 0.0018	1.8 1.4
 METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). 	29 0.0022	2.2 1.7
 METHOD/APPARATUS/PROCEDURE: The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). 		
 The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. (1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). (1) commercial product; less than 3% impurities. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). 	AUXILIARY	INFORMATION
 chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1. (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). (2) distilled over KMnO4 and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). 	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1. May, W.; Chesler, S.; Cram, S.;	chromatography (DCCLC) method was based on generating saturated solu- tions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The con- centration of (1) in the effluent of the generator column was mea- sured by a modification of the coupled column liquid chromato- graphic process that has been	<pre>than 3% impurities. (2) distilled over KMnO₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2) (standard deviation) REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9]	May, W.E.; Wasik, S.P.; Freeman, D.H.		
<pre>(2) Sodium Chloride; NaCl; [7647-14-5]</pre>	Anal. Chem. <u>1978</u> , 50, 997-1000.		
(3) Water; H ₂ O; [7732-18-5]			
VARIABLES: One temperature: 25°C	PREPARED BY:		
Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay		
EXPERIMENTAL VALUES:			
The solubility of chrysene in aqueous	s sodium chloride is		
reported in terms of the Setschenow e	equation:		
log(S _o /S) = K _s C _s			
where;			
S _o is the solubility o	of (1) in water (mg/L)		
S is the solubility of	f (l) in saline solution (mg/L)		
K _s is the Setschenow of	constant (L/mol)		
C _s in the concentration	on of sodium chloride (mol/L)		
evaluating the equation for S over the	ne range of C_ 0-0.7 mol/L,		
$K_{s} = 0.336$ with $S_{o} = 0.0018$.			
The corresponding mass percent and mo	ble fraction x_1 , at salinity =		
35 g(2)/kg sln calculated by the compilers are 1.1 x 10^{-7} g(1)/100 g sln and 8.8 x 10^{-11} .			
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C ₁₈ stationary phase, then a water- acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concen-	 (1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column. ESTIMATED ERROR: temp ± 0.05°C		
tration of (1) was measured with a UV detector.	$K_{s} \pm 0.000$ $S_{o} \pm 0.0001$ REFERENCES:		

COMPONENTS:	EVALUATOR:
<pre>(1) Naphthacene; C₁₈H₁₂; [92-24-0] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for naphthacene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in naphthacene.

TABLE	1.	Quantitati	ive	Solu	ubility	st	udies	of
	N	aphthacene	(1)	in	Water	(2)		

Reference	T/K	Method
Davis et al.(ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The data are also summarized in Table 2 below. The reported values are in poor agreement. The value of Mackay and Shiu (ref 3) being lower than the other reported values (ref 1,2) is preferred as the Tentative solubility at 298K.

TABLE 2. Tentative Solubility Value ofNaphthacene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁸ g(1)/100 g sln	"Best 10 ⁸ g(1)/100 g sln	" value 10 ¹¹ ¤ ₁
298	15^{a} (ref 2), 5.7 (ref 3)	6	5
300	10 ^{<i>a</i>} (ref 1)		

a Values probably high.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Naphthacene; C₁₈H₁₂; [92-24-0] (2) Water; H₂0; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of	naphthacene in water
t/°C	10^6 g(l) L ⁻¹ (2)
27	1.0 ± 0.5
	1.0 ± 0.2

The best value recommended by the authors is 1.0×10^{-6} g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.-0 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 1.0 x 10^{-7} g(1)/ 100 g sln and 7.9 x 10^{-11} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 prepared at Harvard University; m.p. range 341.5-343.0°C; (cf. ref 2). dust-free.
	ESTIMATED ERROR: temp. ± 3°C
	soly. see above
	REFERENCES:
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Naphthacene; C₁₈H₁₂; [92-24-0] (2) Water; H₂O; [7732-18-5]</pre>	Klevens, H.B. J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of naphthacene in water at 25°C was reported to be 6.6 x 10^{-9} mol(1) L⁻¹ sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are 1.5 x 10^{-7} g(1)/100 g sln and 1.2 x 10^{-10} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter- mined by spectra.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y.
(1) Naphthacene; C ₁₈ H ₁₂ ; [92-24-0]	_
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of naphthacene in watter to be 0.00057 mg(l) dm ⁻³ sln and x_1 . The corresponding mass percent calcu	$= 3.7 \times 10^{-11}$.
is 5.7 x 10 ⁻⁸ g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was	 (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	(2) doubly distilled.
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	soly. ± 0.00003 mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

38_418

COMPONENTS :	EVALUATOR:
<pre>(1) Triphenylene; C₁₈H₁₂; [217-59-4] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for triphenylene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in triphenylene.

TABLE 1.	Quantitative	Solu	bility	Studies	of
<u></u>	riphenylene	(1) in	Water	(2)	

Reference	T/K	Method
Davis <i>et al</i> . (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The reported data which are summarized in Table 2 are in excellent agreement. However the solubility values are not sufficiently well characterized, at this stage, to justify Recommending the average value.

TABLE 2. Tentative Solubility Value ofTriphenylene (1) in Water (2)

Т/К	Solubilit	y values	
	Reported values	"Best" va	lue
	10 ⁶ g(1)/100 g sln	10 ⁶ g(1)/100 g sln	10 ⁹ <i>x</i> 1
298	4.28 (ref 2), 4.3 (ref 3)	4.3	3.4
300	3.8 ^{<i>a</i>} (ref 1)	-	-

a Datum not sufficiently well characterized to justify inclusion in "best" values.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. 1950, 54, 283-98.
- 3. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Triphenylene; $C_{18}H_{12}$; [217-59-4] ORIGINAL MEASUREMENTS: (2) Water; H_20 ; [7732-18-5] Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10. VARIABLES: PREPARED BY: One temperature: 27°C M.C. Haulait-Pirson EXPERIMENTAL VALUES: Solubility of triphenylene in water' $\frac{t/°C}{27}$ 10^5 g(1) L ⁻¹ (2) 3.8 ± 0.8 3.6 ± 0.4 4.0 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is 3.8×10^{-5} g(1) L ⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 3.8×10^{-6} g(1)/ 100 g sln and 3.0×10^{-9} .	498	38_419
Cloves, G.H.A. (2) Water; H ₂ O; [7732-18-5] VARIABLES: One temperature: 27°C EXPERIMENTAL VALUES: Solubility of triphenylene in water $\frac{t/°C}{27}$ $\frac{10^5 g(1) L^{-1} (2)}{3.8 \pm 0.8}$ 3.6 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is $3.8 \times 10^{-5} g(1) L^{-1} (2)$. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $3.8 \times 10^{-6} g(1)/$	COMPONENTS :	ORIGINAL MEASUREMENTS:
One temperature: 27°CM.C. Haulait-PirsonEXPERIMENTAL VALUES:Solubility of triphenylene in water $\frac{t/°C}{27}$ $\frac{10^5 g(1) L^{-1} (2)}{3.8 \pm 0.8}$ 273.8 ± 0.83.6 ± 0.44.0 ± 0.4The best value recommended by the authors is $3.8 \times 10^{-5} g(1) L^{-1} (2)$.Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percentand mole fraction, x_1 , calculated by the compiler are $3.8 \times 10^{-6} g(1)/$	20 20	Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64,
EXPERIMENTAL VALUES: Solubility of triphenylene in water $\frac{t/^{\circ}C}{27}$ $\frac{10^{5} g(1) L^{-1} (2)}{3.8 \pm 0.8}$ 3.6 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is $3.8 \times 10^{-5} g(1) L^{-1} (2)$. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_{1} , calculated by the compiler are $3.8 \times 10^{-6} g(1)/$	VARIABLES:	PREPARED BY:
Solubility of triphenylene in water $\frac{t/^{\circ}C}{27} \qquad \frac{10^{5} g(1) L^{-1} (2)}{3.8 \pm 0.8}$ 3.6 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is $3.8 \times 10^{-5} g(1) L^{-1} (2)$. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_{1} , calculated by the compiler are $3.8 \times 10^{-6} g(1)/$	One temperature: 27°C	M.C. Haulait-Pirson
$\frac{t/^{\circ}C}{27}$ $\frac{10^{5} g(1) L^{-1} (2)}{3.8 \pm 0.8}$ 3.6 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is $3.8 \times 10^{-5} g(1) L^{-1} (2)$. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_{1} , calculated by the compiler are $3.8 \times 10^{-6} g(1)/$		envlene in water
3.6 ± 0.4 4.0 ± 0.4 The best value recommended by the authors is 3.8×10^{-5} g(1) L ⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 3.8×10^{-6} g(1)/		-
Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 3.8 x 10 ⁻⁶ g(1)/	27	3.6 ± 0.4
	Assuming that 1.00 L sln = 1.00 kg and mole fraction, x_1 , calculated by	sln the corresponding mass percent

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 197.5-197.9°C; (cf. ref 2).</pre>
nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	(2) dust-free.
Many details are reported in ref 1.	ESTIMATED ERROR:
	temp. ± 3°C soly. see above
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4]	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
2	
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of triphenylene in wat 4.3 x 10^{-5} g(1) L ⁻¹ sln and 1.88 x 1 Assuming that 1.00 L sln = 1.00 kg and mole fraction, x_1 , calculated by 100 g sln and 3.39 x 10^{-9} .	LO ⁻⁷ mol(l) L ⁻¹ sln. sln, the corresponding mass percent
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
The solubility of (1) in (2) was	SOURCE AND PURITY OF MATERIALS: (1) not specified.
determined by shaking small amounts	_
of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations deter-	(2) not specified.
mined by spectra.	
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

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ORIGINAL MEASUREMENTS:
COMPONENTS:
 (1) Triphenylene; C<sub>18</sub>H<sub>12</sub>; [217-59-4]
                                           Mackay, D.; Shiu, W.Y.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
                                           J. Chem. Eng. Data 1977, 22,
                                             399-402.
VARIABLES:
                                          PREPARED BY:
                                           M.C. Haulait-Pirson
One temperature: 25°C
EXPERIMENTAL VALUES:
 The solubility of triphenylene in water at 25°C was reported
to be 0.043 mg(1) dm<sup>-3</sup> sln and x_1 = 3.39 \times 10^{-9}.
 The corresponding mass percent calculated by the compiler
 is 4.3 \times 10^{-6} g(1)/100 g sln.
                                 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
                                           SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) in (2)
                                           (1) Aldrich Chemicals, Eastman
                                               Kodak, or K and K Laboratories,
was vigorously stirred in a 250 mL
flask for 24 hrs. and subsequently
                                               commercial highest grade;
 settled at 25°C for at least 48 hrs.
                                               used as received.
 Then the saturated solution was
decanted and filtered and 50-100 mL
                                           (2) doubly distilled.
extracted with approximately 5 mL
of cyclohexane in a separatory
funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
for analysis. An Aminco-Browman
spectrophotofluorometer (American
Instruments Ltd.) was used for
                                           ESTIMATED ERROR:
analysis. Many details are given
                                           soly. \pm 0.00017 mg(1) dm<sup>-3</sup> sln
in the paper.
                                           (maximum deviation from several
                                           determinations).
                                           REFERENCES:
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38_422

COMPONENTS:	EVALUATOR:
<pre>(1) Octadecane; C₁₈H₃₈; [593-45-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for octadecane (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in octadecane.

	Octadecane (1) in Water (2)	
Reference	T/K	Method
Baker (ref 1)	298-353	radiotracer
Baker (ref 2)	298	radiotracer
Baker (ref 3)	298	not specified
Sutton and Calder (ref 4	1) 298	GLC

TABLE 1. Quantitative Solubility Studies of Octadecane (1) in Water (2)

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the graphical (ref 1) and v/v data (ref 3) reported by Baker which have been excluded from consideration, all the available data (ref 2,4) are summarized in Table 2 below. The reported values are in poor agreement and both are several orders of magnitude higher than would be predicted by an extrapolation of the lower n-alkane solubilities, viz. $\sim 10^{-10}$ g(1)/100 g sln, although the validity of this extrapolation is unknown. Nevertheless it must be recognized that the reported values may be substantially in error and no "best" value has been suggested.

TABLE 2.	Reported Values of the Solubility of)f
	Octadecane (1) in Water (2)	_

<i>Т/</i> К	Reported values ^a 10 ⁷ g(1)/100 g sln	$10^{10} x_1$
298	6 (ref 2), 2.1 (ref 4) 4.2 (ref 2), 1.5 (ref 4)

a No "best" values suggested because of possible errors in data; see text. 501

(continued next page)

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COMPONENTS:

(1) Octadecane; C<sub>18</sub>H<sub>38</sub>; [593-45-3]

(2) Water; H<sub>2</sub>O; [7732-18-5]

University, Perth, W.A., Australia.

June 1986.
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CRITICAL EVALUATION:

(continued)

REFERENCES

- Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints Symposia <u>1956</u>, 1, No.2, 5-17.
- Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u>, 3, No.4, C61-8.
- 3. Baker, E.G. Science 1959, 129, 871-4.
- 4. Sutton, C.; Calder, J.A. Environ. Sci. Technol. 1974, 8, 654-7.

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COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Baker, E.G.		
(2) Water; H ₂ O; [7732-18-5]	Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia <u>1956</u> , 1, N°2, 5-17.		
VARIABLES:	PREPARED BY:		
Temperature: 5-80°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
The authors reported that the solubil increases from about 55 ppb by weight this amount at 80°C. A graph reporti of the reciprocal absolute temperatur	: at room temperature to twice ang the mole fraction x_1 a function		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Tritio-octadecane was used as radio- active tracer. 0.01 of active (1) was shaken with (2); the mixture was filtered through a 0.05 μ m fil- ter; 0.01 mL of filtrate was vaporized in hot oxygen and passed over CuO at 600°C; the H ₂ O-T ₂ O derived from the vaporized solvent as well as from the combusted (1) was trapped at -78°C; the melted ice was reduced by Zn and the gas was counted. Many details are given in the paper.	 (1) tritio-octadecane prepared by hydrogenating octadecene-1 with tritium; 100 curies of tritium were introduced per mole of (1). (2) distilled. ESTIMATED ERROR: not specified. 		
	REFERENCES:		

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504
                                                                                    38 424
COMPONENTS:
                                              ORIGINAL MEASUREMENTS:
  (1) Octadecane; C<sub>18</sub>H<sub>38</sub>; [593-45-3]
                                               Baker, E.G.
                                               Am. Chem. Soc., Div. Petrol.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
                                                 Chem., Preprints 1958, 3, N°4,
                                                 C61-8.
VARIABLES:
                                              PREPARED BY:
                                               M.C. Haulait-Pirson
 One temperature: 25°C
EXPERIMENTAL VALUES:
 The solubility of octadecane-1,2-H<sup>3</sup> in water at 25°C was reported
 to be 6 x 10^{-9} g(1)/g(2) and that of octadecane-1-C<sup>14</sup> 5.7 x 10^{-9}
 q(1)/q(2).
 The corresponding mass fraction and mole fraction, x_1, calculated by
 the compiler are 6 \times 10^{-7} g(1)/100 g sln and 4 \times 10^{-10}.
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOU Tritiated or carbon-14 labeled (1) (1 was used as tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect (2 the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

- (1) Octadecane-1,2-H³ from Tracer Lab.; percolated through silica gel. Octadecane-1-C¹⁴ from Nuclear Instrument and Chemical Corporation; used as received.
- (2) distilled.

ESTIMATED ERROR:

soly. 20% (standard deviation from
17 replicate runs).

REFERENCES:

 Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia <u>1956</u>, 1, N°2, 5.

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50_425			
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3]	Baker, E.G.		
(2) Water; H ₂ O; [7732-18-5]	Science <u>1959</u> , 129, 871-4.		
	· · · · · · · · · · · · · · · · · · ·		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	F. Kapuku		
EXPERIMENTAL VALUES:			
The solubility of octadecane in water 7.75 x 10^{-7} mL(1)/100 mL(2).	r at 25°C was reported to be		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
not specified.	not specified.		
	ESTIMATED ERROR:		
	not specified.		
	-		
	REFERENCES :		

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) Octadecane; C ₁₈ H ₃₈ ; [593-45-3] (2) Water; H ₂ O; [7732-18-5]	Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.		
VARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			

The solubility of octadecane in water at 25°C was reported to be 2.1 x 10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 , of 1.5 x 10^{-10} .

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled. ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16% REFERENCES:			

COMPONENTS: (1) Octadecane; C₁₈H₃₈; [593-45-3] (2) Seawater (2) Seawater (3) Seawater (4) Seawater (5) S

VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of octadecane in seawater was reported to be 8 x 10^{-8} g(1)/100 g sln and $x_1 = 5 \times 10^{-11}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana-	<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre>
lyzed by gas chromatography.	ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

508	38_428
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Methylbenz[a]anthracene; C₁₉H₁₄; [2498-77-3]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of 1-methylber	nz[a]anthracene in water
t/°C	$10^5 g(1) L^{-1} (2)$
27	5.5 ± 0.2
	5.4 ± 0.4
	5.5 ± 0.2
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	 (1) prepared at Harvard University; m.p. range 138.5-139.0°C (cf. ref 2). (2) dust-free.
Many details are reported in ref 1.	ESTIMATED ERROR:
	temp. ± 3°C soly. see above
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc 1940, 62, 3086.</pre>

38_429	509
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 9-Methylbenz[a]anthracene; C₁₉H₁₄; [2381-16-0]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of 9-methylbenz[a]anth was reported to be 6.6 x 10^{-5} g(1) L (Two identical results have been obta With the assumption that 1.00 L sln mass percent and mole fraction, x_1 , c 6.6 x 10^{-6} g(1)/100 g sln and 4.5 x 1	(2). (ined) = 1.00 kg sln, the corresponding alculated by the compiler are
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained	 (1) prepared at Harvard University; m.p. range 138.0-138.8°C (cf. ref 2). (2) dust-free.

articles of the relation and equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1. ESTIMATED ERROR: temp. ± 3°C soly. ± 0.3 x 10⁻⁵ g(1) dm⁻³(2) REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. Davis W.W. With With the solution (1) 101. (2) 101.

2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.

38_430

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) 10-Methylbenz[a]anthracene; C₁₉H₁₄; [2381-15-9]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 27°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:	I		
The solubility of 10-methylbenz[a]and was reported to be 5.5 x 10^{-5} g(1) L (Four identical results have been obt With the assumption that 1.00 L slr mass percent and mole fraction, x_1 , o 5.5 x 10^{-6} g(1)/100 g sln and 4.1 x 1	(2). tained) h = 1.00 kg sln, the corresponding calculated by the compiler are		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<pre>SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 140.0-140.5°C (cf. ref 2). (2) dust-free. (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. ± 0.5 x 10⁻⁵ g(1) dm⁻³(2) REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>		

COMPONENTS :			
	ORIGINAL MEASUREMENTS:		
(1) 5-Methylchrysene; C ₁₉ H ₁₄ ; [3697-24-3]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.		
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.		
VARIABLES:	PREPARED BY:		
One temperature: 27°C	M.C. Haulait-Pirson		
EXPERIMENTAL VALUES:			
Solubility of 5-methylchry	sene in water		
t/°C 10	5 g(1) ${}_{L}^{-1}$ (2)		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			
mass percent and mole fraction, x_1 , calculated by the compiler are 6.2 x 10^{-6} g(1)/100 g sln and 4.6 x 10^{-9} .			
AUXILIARY	AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	INFORMATION		
	SOURCE AND PURITY OF MATERIALS:		
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.			

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COMPONENTS :	EVALUATOR:
<pre>(1) Benzo[a]pyrene; C₂₀H₁₂; [50-32-8] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for benzo[a]pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in benzo[a]pyrene.

TABLE	E 1. Quantitative		lubility	Studies	of
	Benzo[a]py	rene (1)	in Water	(2)	

Reference	Т / К	Method
Davis et al. (ref 1)	300	nephelometric
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. It can be seen from Table 2 that the reported solubility values are in good agreement, given that they have been measured at slightly different temperatures. However, further studies are required before any data can be Recommended.

TABLE 2.TentativeSolubilityValuesofBenzo[a]pyrene(1)inWater(2)

T/K		Solubility values	
	Reported values	"Best" va	
	10 ⁷ g(1)/100 g sln	10 ⁷ g(1)/100 sln	$10^{10} x_1$
298	3.8 (ref 2)	3.8	2.7
300	4.0 (ref 1)	4.0	2.9

REFERENCES

 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.

2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u>, 22, 399-402.

38_433

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
Solubility of b	penzo[a]pyrene in water
- t/°C	$10^{6} g(1) L^{-1} (2)$
<u> </u>	
27	3.0 ± 0.5

4.5 ± 0.5 4.0 ± 0.1 4.0 ± 0.5

3.5 ± 0.5
The best value recommended by the authors is 4.0 x 10^{-6} g(1) L ⁻¹ (2).
With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding
mass percent and mole fraction calculated by the compiler are 4.0×10^{-7} g(l)/100 g sln and 2.9 x 10^{-10} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	 (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free.
Many details are reported in ref 1.	ESTIMATED ERROR:
	temp. ± 3°C soly. see above
	REFERENCES :
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

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COMPONENTS:
                                          ORIGINAL MEASUREMENTS:
 (1) Benzo[a]pyrene; C<sub>20</sub>H<sub>12</sub>;
                                           Mackay, D.; Shiu, W.Y.
      [50 - 32 - 8]
                                           J. Chem. Eng. Data 1977, 22,
                                              399-402.
 (2) Water; H<sub>2</sub>O; [7732-18-5]
VARIABLES:
                                          PREPARED BY:
                                           M.C. Haulait-Pirson
 One temperature: 25°C
EXPERIMENTAL VALUES:
 The solubility of benzo[a]pyrene in water at 25°C was reported
 to be 0.0038 mg(1) dm<sup>-3</sup> sln and x_1 = 2.73 \times 10^{-10}.
 The corresponding mass percent calculated by the compiler
 is 3.8 \times 10^{-7} q(1)/100 q sln.
                                 AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
                                           SOURCE AND PURITY OF MATERIALS:
 A saturated solution of (1) in (2)
                                            (1) Aldrich Chemicals, Eastman
 was vigorously stirred in a 250 mL
                                                Kodak, or K and K Laboratories,
                                                commercial highest grade;
 flask for 24 hrs. and subsequently
 settled at 25°C for at least 48 hrs.
                                                used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
                                            (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
 funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
 for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
                                           ESTIMATED ERROR:
 analysis. Many details are given
                                           soly. \pm 0.00031 mg(1) dm<sup>-3</sup> sln
 in the paper.
                                            (maximum deviation from several
                                           determinations).
                                           REFERENCES:
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38_435

56_455	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8]	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of benzo[a]pyrene in to be 0.13 µg/L. The corresponding mass percent and m	
by the compilers are 1.3×10^{-8} g(1) assuming a solution density of 1.004	$/100 \text{ g sln and } 9.5 \times 10^{-12}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the	Not given.
solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken	
for analysis. The solution was cen- trifuged twice at 7000 g to remove	ESTIMATED ERROR:
suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma-	temp. ± 1°C soly. ± 0.008 type of error not specified
tography. Spectrometric analysis	REFERENCES :
of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.	 Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Neftekhimiya <u>1973</u>,
<u> </u>	

COMPONENTS: (1) Benzo[e]pyrene; C ₂₀ H ₁₂ ; [192-97-2] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Schwarz, F.P. J. Chem. Eng. Data <u>1977</u> , 22, 273-7.
VARIABLES:	PREPARED BY:
Temperature: 8.6-31.7°C	A. Maczynski

EXPERIMENTAL VALUES:

	Solubility of benzo	e]pyrene in water	
t/°C	10 ⁸ mol(1) L	10 ⁷ g(1)/100 g sln (compiler)	10 ¹⁰ x1 (compiler)
8.6	1.29 ± 0.07	3.25	2.32
14.0	1.42 ± 0.05	3.58	2.56
17.0	1.76 ± 0.13	4.44	3.17
17.5	1.56 ± 0.08	3.94	2.81
20.0	1.82 ± 0.09	4.59	3.28
20.2	1.90 ± 0.14	4.79	3.42
23.0	2.01 ± 0.20	5.07	3.62
23.2	2.12 ± 0.10	5.35	3.82
29.2	2.55 ± 0.02	6.43	4.59
31.7	2.70 ± 0.15	6.81	4.86

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Two methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectro- fluorimetry method was used.	 source not specified; better than 99 mole%, by glc; used as received. distilled over KMnO4 and NaOH and passed through a Sephadex column.
The sealed fluorescence cells con- tained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.	ESTIMATED ERROR: temp. ± 0.1°C soly. see above REFERENCES:

38_437

50_457			5
COMPONENTS :		EVALUATOR:	<u></u>
 Benzo[e]pyrene; [192-97-2] Seawater 	C ₂₀ H ₁₂ ;	D.G. Shaw Institute of M University of J Fairbanks, Ala	Alaska
		December 1982	
CRITICAL EVALUATION:			
The solubility of be reported in two work		in seawater (2)	at 298 K has been
Authors	Method	Salinity g salts/kg sln	10 ⁷ g(1)/100 g sln
Krasnoshchekova <i>et a</i> (ref 1)	<pre>1. spectral</pre>	6	1.79
Schwarz (ref 2)	uv spectral	30	3.32
т/к	Y OF BENZO[E]PYRE TENTATIVE g salts/k	VALUES	g(l)/100 g sln
298	6		1.79
298	30		3.32
REFERENCES			
 Krasnoshchekova, <i>Topl.</i> <u>1977</u>, 11, 		Yu.A; Gubergrits	, M.Ya. Khim. Tverd.
2. Schwarz, F.P. J	. Chem. Eng. Data	<u>1977</u> , 22, 273-	7.

COMPONENTS: (1) Benzo[e]pyrene; C ₂₀ H ₁₂ ; [192-97-2]	ORIGINAL MEASUREMENTS:
	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of Benzo[e]pyrene in to be 1.83 μ g/L.	salt water was reported
The corresponding mass percent and m by the compilers are 1.79 x 10 ⁻⁷ g(1 assuming a solution density of 1.004	$)/100 \text{ g sln and } 1.34 \times 10^{-10}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.</pre>	ESTIMATED ERROR:

	ORIGINAL MEASUREMENTS:
<pre>(1) Benzo[e]pyrene; C₂₀H₁₂; [192-97-2]</pre>	Schwarz, F.P.
<pre>(2) Sodium chloride; NaCl; [7647-14-5]</pre>	J. Chem. Eng. Data <u>1977</u> , 22, 273 - 7.
(3) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 8.9-30.2°C	W.Y. Shiu, D. Mackay
Salinity: 30 g(2)/kg sln	-
EXPERIMENTAL VALUES:	
Solubility of benzo[e]py	rene in 0.5 mol(2)/L
<u>t/°C</u>	10 ⁸ mol(l)/L sln
8.9	0.82
10.8	0.88
15.6	1.01
17.0	1.01
19.2	1.04
21.7	1.13
25.3	1.35
27.1	1.42
30.2	1.66
The corresponding mass percent and calculated by the compilers are 3	d mole fraction, x_1 , at 25.3°C .32 x 10 ⁻⁷ g(1)/100 g sln and
The corresponding mass percent and calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ .	d mole fraction, x_1 , at 25.3°C .32 x 10 ⁻⁷ g(1)/100 g sln and
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ .	d mole fraction, x_1 , at 25.3°C .32 x 10 ⁻⁷ g(l)/100 g sln and INFORMATION
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ .	$.32 \times 10^{-7} \text{ g(l)/l00} \text{ g sln and}$
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in	.32 x 10 ⁻⁷ g(l)/100 g sln and INFORMATION
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea-	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS;
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %,
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade.
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea-	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade.
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio-	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade.
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]-	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR:
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal.	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author)
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMn04 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal.	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)
calculated by the compilers are 3 2.44 x 10 ⁻¹⁰ . AUXILIARY METHOD/APPARATUS/PROCEDURE: The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption mea- surements. In the fluorescence method, saturated solution was pre- pared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell contain- ing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was mea- sured at 410 and 265 nm. The Spec- trofluorimeter employed a ratio- photon counting mode where benzo[e]- pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore provide an absolute solubility scale for the	.32 x 10 ⁻⁷ g(1)/100 g sln and INFORMATION SOURCE AND PURITY OF MATERIALS: Benzo[e]pyrene: purity > 99 mole %, Sodium chloride: reagent grade, Water: distilled over a KMnO4 - NaOH solution and passed through a Sephadex column, Cyclohexane: reagent grade. ESTIMATED ERROR: Solubility ± 19.5% (author) Temperature ± 0.1°C (author)

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COMPONENTS:
                                               ORIGINAL MEASUREMENTS:
                                                Mackay, D.; Shiu, W.Y.
  (1) Perylene; C<sub>20</sub>H<sub>12</sub>; [198-55-0]
  (2) Water; H<sub>2</sub>O; [7732-18-5]
                                                J. Chem. Eng. Data <u>1977</u>, 22,
                                                   399-402.
VARIABLES:
                                               PREPARED BY:
                                                M.C. Haulait-Pirson
 One temperature: 25°C
EXPERIMENTAL VALUES:
 The solubility of perylene in water at 25°C was reported
 to be 0.0004 mg(1) dm<sup>-3</sup> sln and x_1 = 2.83 \times 10^{-11}.
 The corresponding mass percent calculated by the compiler
 is 4 \times 10^{-8} g(1)/100 g sln.
                                    AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
                                               SOURCE AND PURITY OF MATERIALS:
                                                (1) Aldrich Chemicals, Eastman
 A saturated solution of (1) in (2)
 was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently
                                                     Kodak, or K and K Laboratories,
                                                     commercial highest grade;
 settled at 25°C for at least 48 hrs.
                                                     used as received.
 Then the saturated solution was
 decanted and filtered and 50-100 mL
                                                (2) doubly distilled.
 extracted with approximately 5 mL
 of cyclohexane in a separatory
 funnel. After shaking for 2 hrs.
 the cyclohexane extract was removed
for analysis. An Aminco-Browman
 spectrophotofluorometer (American
 Instruments Ltd.) was used for
                                               ESTIMATED ERROR:
 analysis. Many details are given
                                                soly. \pm 2 x 10<sup>-5</sup> mg(1) dm<sup>-3</sup> sln (maximum deviation from several
 in the paper.
                                                determinations).
                                               REFERENCES:
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38_441

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cholanthrene; C ₂₀ H ₁₄ ; [479-23-2]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

The solubility of cholanthrene in water at 27°C was reported to be $3.5 \times 10^{-6} \text{ g(1) L}^{-1}$ (2). (Two identical results were obtained). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $3.5 \times 10^{-7} \text{ g(1)/100 g sln and } 2.5 \times 10^{-10}$.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 170.1-170.6°C; (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. ± 0.5 x 10 ⁻⁶ g(1) dm ⁻³ (2) REFERENCES:
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 7,12-Dimethylbenz[a]anthracene;	Mackay, D.; Shiu, W.Y.	
C ₂₀ H ₁₆ ; [57-97-6]	J. Chem. Eng. Data <u>1977</u> , 22,	
(2) Water; H ₂ O; [7732-18-5]	399-402.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C was reported to be 0.061 mg(1) dm ⁻³ sln and $x_1 = 4.26 \times 10^{-9}$. The corresponding mass percent calculated by the compiler is 6.1 $\times 10^{-6}$ g(1)/100 g sln.		
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	 (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.0006 mg(1) dm⁻³ sln (maximum deviation from several determinations). REFERENCES: 	

COMPONENTS:

38_443

COMPONENTS :	ORIGINAL MEASUREMENTS:	
<pre>(1) 9,10-Dimethylbenz[a]anthracene; C₂₀H₁₆; [56-56-4]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.	
VARIABLES:	PREPARED BY:	
One temperature: 27°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of 9,10-dimethylbe	enz[a]anthracene in water	
t/°C	10^5 g(1) L ⁻¹ (2)	
The best value recommended by the aut With the assumption that 1.00 L slm mass percent and mole fraction, x_1 , o 4.3 x 10 ⁻⁶ g(1)/100 g sln and 3.0 x 1	a = 1.00 kg sln, the corresponding calculated by the compiler are	
AUXILIARY INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	

ESTIMATED ERROR: temp. ± 3°C soly. see above

REFERENCES:

1.		Parker Soc. <u>1</u>	
2.	J. An	Krahl, m. Chem	Cloves, <u>1940</u> ,

meter model 100-mm was employed. Many details are reported in ref 1.

COMPONENTS:		
	ORIGINAL MEASUREMENTS:	
<pre>(1) 10-Ethylbenz[a]anthracene; C_{20^H16}; [14854-08-1]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108–10.	
VARIABLES:	PREPARED BY:	
One temperature: 27°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of 10-ethylbenz[a]anthracene in water		
t/°C	$10^5 g(1) L^{-1} (2)$	
The best value recommended by the aut With the assumption that 1.00 L slumass percent and mole fraction, x_1 , 6 4.5 x 10 ⁻⁶ g(1)/100 g sln and 3.2 x 3	n = 1.00 kg sln, the corresponding calculated by the compiler are	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further	<pre>(1) prepared at Harvard University; m.p. range 112.4-112.8°C (cf. ref 2).</pre>	

38_445

COMPONENTS:	ORIGINAL MEASUREMENTS:	
	OKIGINAL MERSUREMENTS.	
(1) Eicosane; C ₂₀ H ₄₂ ; [112-95-8]	Sutton, C.; Calder, J.A.	
(2) Water; H ₂ O; [7732-18-5]	Environ. Sci. Technol. <u>1974</u> , 8, 654-7.	
VARIABLES:	PREPARED BY:	
One temperature: 25°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
The solubility of eicosane in water at 25°C was reported to be 1.9 x 10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 , of 1.1 x 10^{-10} .		
	INFORMATION	
METHOD/APPARATUS/PROCEDURE:		
	SOURCE AND PURITY OF MATERIALS:	
175 mg (1) were equilibrated with	(1) Analabs Inc., 99+%.	
700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then	(2) doubly distilled.	
allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore		
filter, then extracted three times with 10-mL portions of hexane con- taining an internal standard. The concentration of (1) was determined		
by injection of the hexane extract	ESTIMATED ERROR:	
into a dual column gas chromatograph equipped with flame ionization de- tectors.	temp. ± 0.1°C soly. ± 16%	
	REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Eicosane; C ₂₀ H ₄₂ ; [112-95-8] (2) Seawater	Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	PREPARED BY: P.A. Meyers and D. Shaw

The solubility of eicosane in seawater was reported to be $8 \times 10^{-8} \text{ g(1)/100 g sln and } x_1 = 5 \times 10^{-11}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^{\circ}$ C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana-	<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre>
lyzed by gas chromatography.	ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 5-Methylbenzo[a]pyrene; C_{21H14}; [2319-96-2]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.	
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.	
VARIABLES:	PREPARED BY:	
One temperature: 27°C	M.C. Haulait-Pirson	
EXPERIMENTAL VALUES:		
Solubility of 5-methylben t/°C	zo[a]pyrene in water 10 ⁷ g(1) L ⁻¹ (2)	
27	8 ± 2 10 ± 4 8 ± 2	
The best value recommended by the authors is 8×10^{-7} g(1) L ⁻¹ (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 8×10^{-8} g(1)/100 g sln and 6×10^{-11} .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) prepared at Harvard University; m.p. range 216.6-217.3°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V.	

COMPONENTS:	EVALUATOR:
<pre>(1) 3-Methylcholanthrene; C₂₁H₁₆; [56-49-5] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.
	June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 3-methylcholanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data are available on the solubility of water in 3-methylcholanthrene.

TABLE 1.	Quantitative	Solub	ility	Stud	lies	of
<u>3-Met</u>	hylcholanthren	e (1)	in Wa	ater	(2)	

T/K	Method
300	nephelometric
298	spectrofluorometric
	300

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. Unfortunately, the available data, obtained at slightly different temperatures are in poor agreement. Although the values of Mackay and Shiu (ref 2) are generlly more reliable than those of Davis *et al.* (ref 1) the system is not sufficiently well-characterized to justify a preference at this stage and no "best" values have been nominated.

TABLE 2. Reported Solubility Values of3-Methylcholanthrene (1) in Water (2)

T/K	Reported va	Reported values ^a		
	10 ⁷ g(1)/100 g sln	$10^{10} x_1$		
298	2.9 (ref 2)	1.9 (ref 2)		
300	1.5 (ref 1)	1.0 (ref 1)		

a No "best" values nominated because of uncertainties in the available data, see text.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methylcholanthrene; C_{21^H16}; [56-49-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

Solubility	of	3-methylcholanthrene in water
t/°C		10^{6} q(1) L ⁻¹ (2)

27 0		•
27	1.3	
	1.8	
	1.8	

The best value recommended by the authors is $1.5 \times 10^{-6} \text{ g(1) L}^{-1}$ (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $1.5 \times 10^{-7} \text{ g(1)}/100 \text{ g sln and } 1.0 \times 10^{-10}$.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed.	 SOURCE AND PURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 175.3-177.1°C; (cf. ref 2). (2) dust-free. 		
Many details are reported in ref 1.	ESTIMATED ERROR: temp. \pm 3°C soly. \pm 0.3 x 10 ⁻⁶ g(1) dm ⁻³ (2)		
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>		

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ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1977</u> , 22, 399-402.				
PREPARED BY: M.C. Haulait-Pirson				
One temperature: 25°C M.C. Haulait-Pirson EXPERIMENTAL VALUES: The solubility of 3-methylcholanthrene in water at 25°C was reported to be 0.0029 mg(1) dm ⁻³ sln and $x_1 = 1.92 \times 10^{-10}$. The corresponding mass percent calculated by the compiler is 2.9 x 10 ⁻⁷ g(1)/100 g sln.				
INFORMATION				
<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.000021 mg(1) dm⁻³ sln (maximum deviation from several determinations).</pre>				

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; C ₂₂ H ₁₂ ;	Mackay, D.; Shiu, W.Y.
[191-24-2]	J. Chem. Eng. Data 1977, 22,
	399-402.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
	M.C. Madrart Filson
EXPERIMENTAL VALUES:	
The solubility of benzo[ghi]perylene	in water at 25 °C was reported
to be 0.00026 mg(1) dm ⁻³ sln and x_1	$= 1.73 \times 10^{-11}$.
-	
The corresponding mass percent calcu	lated by the compiler
is 2.6 x 10^{-8} g(1)/100 g sln.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	
A saturated solution of (1) in (2)	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman
was vigorously stirred in a 250 mL	Kodak, or K and K Laboratories,
flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs.	commercial highest grade; used as received.
Then the saturated solution was	
decanted and filtered and 50-100 mL extracted with approximately 5 mL	(2) doubly distilled.
of cyclohexane in a separatory	
funnel. After shaking for 2 hrs. the cyclohexane extract was removed	
for analysis. An Aminco-Browman	
spectrophotofluorometer (American Instruments Ltd.) was used for	ESTIMATED ERROR:
analysis. Many details are given in the paper.	$soly. \pm 10^{-5} mg(1) dm^{-3} sln$
in the paper.	(maximum deviation from several determinations).
	determinations).
	REFERENCES:

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COMPONENTS :	ORIGINAL MEASUREMENTS:
 (1) Benzo[b]triphenylene; C₂₂H₁₄; [215-58-7] (2) Salt Water 	<pre>Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u>, 11, 133-6.</pre>
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	

The solubility of benzo[b]triphenylene in salt water was reported to be 27.84 $\mu\text{g/L}.$

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 2.719 x 10^{-6} g(1)/100 g sln and 1.841 x 10^{-9} assuming a solution density of 1.004 kg/L.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was cen- trifuged twice at 7000 g to remove suspended particles. The hydro- carbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chroma- tography. Spectrometric analysis of an octane solution of the hydro- carbon was done using the quasili- near luminescence spectra.</pre>	ESTIMATED ERROR:

COMPONENTS:	EVALUATOR:
<pre>(1) Dibenz[a,h]anthracene; C_{22^H14}; [58-70-3] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for dibenz[a,h]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data are available for the solubility of water in dibenz[a,h]anthracene.

TABLE 1. Quantitative Solubility Studies ofDibenz[a,h]anthracene (1) in Water (2)

T/K	Method
300	nephelometric
298	spectrophotometric
	300

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. The two reported values, although obtained at slightly different temperatures, are in excellent agreement. Nevertheless there are insufficient data and the system is insufficiently well-characterized to justify a higher than Tentative classification.

TABLE 2. Tentative Solubility Values of Dibenz[a,h]anthracene (1) in Water (2)

<i>Т</i> / К	Solubility values		
	Reported values	"Best" val	
	10 ⁸ g(1)/100 g sln	10 ⁸ g(l)/100 g sln	$10^{11} x_1$
298	5.84 (ref 2)	6	4
300	5 (ref 1)	5	3

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u>, 64, 108-10.
- 2. Klevens, H.B. J. Phys. Chem. <u>1950</u>, 54, 283-98.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Dibenz[a,h]anthracene; C_{22^H14}; [58-70-3]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	

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The solubility of dibenz[a,h]anthracene in water at 27°C was reported to be 5 x 10^{-7} g(1) L<sup>-1</sup> (2).
(Two identical results have been obtained)
With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5 x 10^{-8} g(1)/100 g sln and 3 x 10^{-11}.
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AUXTLTARY	INFORMATION
AUVILIAUI	INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<pre>(1) Eastman Kodak Company; purified; m.p. range 266.6-266.9°C or Hoffman La Roche; m.p. range 262.7-264°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C7 soly. ± 10⁻⁷ g(1) dm⁻³(2) REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940,</pre>
	62, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Dibenz[a,h]anthracene; C₂₂H₁₄; [58-70-3]</pre>	Klevens, H.B.
(2) Water; H ₂ O; [7732-18-5]	J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of dibenz[a,h]anthrace to be 2.15 x 10^{-9} mol(1) L ⁻¹ sln. With the assumption that 1.00 L sln mass percent and mole fraction, x_1 , c 5.84 x 10^{-8} g(1)/100 g sln and 3.88 x	= 1.00 kg sln, the corresponding alculated by the compiler are
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long	 not specified. not specified
as three nonths. Aliquots were removed and concentrations deter- mined by spectra.	(2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:
·	

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ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. <i>Khim. Tverd. Topl.</i> <u>1977</u> , <i>11</i> , 133-6.	
Yu.A.; Gubergrits, M.Ya. Khim. Tverd. Topl. <u>1977</u> , 11,	
PREPARED BY:	
M. Kleinschmidt and D. Shaw	
cene in salt water was reported	
The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 2.064 x 10^{-6} g(1)/100 g sln and 1.397 x 10^{-9} assuming a solution density of 1.004 kg/L.	
INFORMATION	
SOURCE AND PURITY OF MATERIALS:	
Not given. ESTIMATED ERROR: temp. ± 1°C soly. ± 1.14 type of error not specified REFERENCES: 1. Krasnoshchekova, R.Ya; Guber- grits, M.Ya. Nejtekhimiya <u>1973</u> , 13,	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Dibenz[a,j]anthracene; C_{22^H14}; [224-41-9]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

	a,j]anthracene in water 10 ⁵ g(1) L ⁻¹ (2)
<i>t/°C</i>	10 ⁻ g(1) L - (2)
27	1.1 ± 0.1
	1.0 ± 0.2 1.3 ± 0.2
The best value recommended by the aut With the assumption that 1.00 L slm mass percent and mole fraction, x_1 , c 1.2 x 10^{-6} g(1)/100 g sln and 7.8 x 1	n = 1.00 kg sln, the corresponding calculated by the compiler are
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) prepared at the Ohio State University; m.p. range 198.0-198.4°C (cf. ref 2). (2) dust-free.
	temp. ± 3°C soly. see above
	<pre>REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.</pre>

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Components :	ORIGINAL MEASUREMENTS:
<pre>(1) Dibenz[a,j]anthracene; C₂₂H₁₄; [224-41-9]</pre>	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.
(2) Salt Water	Khim. Tverd. Topl. <u>1977</u> , 11, 133-6.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M. Kleinschmidt and D. Shaw
Salinity: 6 g/kg sln (ref. 1)	
EXPERIMENTAL VALUES:	
The solubility of dibenz[a,j]anthrad	rene in salt water was reported
to be 10.544 µg/L.	
The corresponding mass percent and m by the compilers are 1.029 x 10 ⁻⁶ g assuming a solution density of 1.004	$(1)/100 \text{ g sln and } 6.970 \times 10^{-10}$
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
<pre>1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distribu- ted over the inside surface of a 1- L round-bottomed flask; the ace- tone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried resi- due, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended par- ticles. The hydrocarbon was ex- tracted with benzene and concen- trated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear lumi- nescence spectra.</pre>	ESTIMATED ERROR: temp. ± 1°C soly. ± 1.05

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) Picene; C₂₂H₁₄; [213-46-7] (2) Water; H₂O; [7732-18-5]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

The solubility of picene in water at 27°C was reported to be 2.5 x 10^{-6} g(1) L⁻¹ (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 2.5 x 10^{-7} g(1)/100 g sln and 1.6 x 10^{-10} .

AUXILIARY	INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduc- tion in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	 (1) prepared at the Ohio State University; m.p. range 363.5-364.5°C; (cf. ref 2). (2) dust-free.
	ESTIMATED ERROR:
	temp. \pm 3°C soly. \pm 0.5 x 10 ⁻⁶ g(1) dm ⁻³ (2)
	REFERENCES:
	 Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. 1942, 64, 101. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. 1940, 62, 3086.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 10-Butylbenz[a]anthracene; C₂₂H₂₀; [31632-63-0]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	•]
Solubility of 10-butylbe	enz[a]anthracene in water
 <i>t/</i> °C	$10^{6} g(1) L^{-1} (2)$
27	7 ± 0.7
27	7 ± 0.7
	7 ± 0.7
	8 ± 1
The best value recommended by the aut With the assumption that 1.00 L slr mass percent and mole fraction, x_1 , c	8 ± 1 thors is 8.0×10^{-6} g(1) L ⁻¹ (2). h = 1.00 kg sln, the corresponding calculated by the compiler are
With the assumption that 1.00 L slr	8 ± 1 thors is 8.0×10^{-6} g(1) L ⁻¹ (2). h = 1.00 kg sln, the corresponding calculated by the compiler are
With the assumption that 1.00 L slr mass percent and mole fraction, x_1 , c 8.0 x 10^{-7} g(1)/100 g sln and 5.1 x 1	8 ± 1 thors is 8.0×10^{-6} g(1) L ⁻¹ (2). n = 1.00 kg sln, the corresponding calculated by the compiler are 0^{-10} .
With the assumption that 1.00 L slr mass percent and mole fraction, x_1 , c 8.0 x 10^{-7} g(1)/100 g sln and 5.1 x 1	8 ± 1 thors is 8.0×10^{-6} g(1) L ⁻¹ (2). h = 1.00 kg sln, the corresponding calculated by the compiler are

REFERENCES:

Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc. <u>1942</u>, 64, 101.
 Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. J. Am. Chem. Soc. <u>1940</u>, 62, 3086.

Components :	ORIGINAL MEASUREMENTS:
<pre>(1) 7-Pentylbenz[a]anthracene; C₂₃H₂₂; [63019-00-1]</pre>	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1942</u> , 64, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
	benz[a]anthracene in water
t/°C	$\frac{10^7 \text{ g(1) } \text{L}^{-1} \text{ (2)}}{10^7 \text{ g(1) } \text{L}^{-1} \text{ (2)}}$
27	9 ± 1
	8 ± 3
	8 ± 2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelo- metrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colori- meter model 100-mm was employed. Many details are reported in ref 1.	<pre>(1) prepared at Harvard University; m.p. range 82.6-83.3°C (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. J. Am. Chem. Soc, 1942, 64,</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Coronene; C ₂₄ H ₁₂ ; [191-07-1]	Mackay, D.; Shiu, W.Y.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data <u>1977</u> , 22, 399-402.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of coronene in water a to be 0.00014 mg(1) dm ⁻³ sln and $x_1 = \frac{1}{2}$	
The corresponding mass percent calcu is 1.4 x 10 ⁻⁸ g(1)/100 g sln.	lated by the compiler
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman	<pre>SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled.</pre>
spectrophotofluorometer (American Instruments Ltd.) was used for	
analysis. Many details are given in the paper.	ESTIMATED ERROR: soly. $\pm 2 \times 10^{-5}$ mg(1) dm ⁻³ sln (maximum deviation from several determinations).
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexacosane; C ₂₆ H ₅₄ ; [110-82-7] (2) Water; H ₂ O; [7732-18-5]	Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	•

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The solubility of hexacosane in water at 25°C was reported to be 1.7 \times 10^{-7} \text{ g(1)/100 g(2)} corresponding to a mole fraction x_1, of 0.8 x 10^{-10}.
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AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: 175 mg (1) were equilibrated with 700 mL (2) in closed flasks by sha- king on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane con-	SOURCE AND PURITY OF MATERIALS: (1) Analabs Inc., 99+%. (2) doubly distilled.
taining an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization de- tectors.	ESTIMATED ERROR: temp. ± 0.1°C soly. ± 16%
	REFERENCES :

38_465

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexacosane; C ₂₆ H ₅₄ ; [630-01-3] (2) Seawater	Sutton, C.; Calder, J.A. Environ. Sci. Technol. <u>1974</u> , 8, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw
EXPERIMENTAL VALUES:	
The solubility of hexacosane in seawater was reported to be $1 \times 10^{-8} \text{ g(l)/100 g sln and } x_1 \approx 6 \times 10^{-12}$.	

AUXILIARY	INFORMATION

METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The com- ponents were equilibrated by gentle shaking for 12 hrs at $25.0 \pm 0.1^{\circ}$ C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extrac- ted three times with hexane and ana- lyzed by gas chromatography.	<pre>Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Na- tural n-alkane levels too low to cause interference.</pre>
	ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental er- ror of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter. REFERENCES:

	38_466
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Hexatriacontane; C₃₆H₇₄; [630-06-8]</pre>	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Am. Chem. Soc., Div. Petrol. Chem., Preprints <u>1958</u> , 3, N°4, C61-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EXPERIMENTAL VALUES:	
The solubility of hexatriacontane-18, reported to be $1.7 \times 10^{-9} g(1)/g(2)$.	
The corresponding mass percent and mothe compiler are $1.7 \times 10^{-7} g(1)/100$	le fraction, x_1 , calculated by g sln and 6.1 x 10^{-11} .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Carbon-14 labeled (1) was used as tracer. The technique of preparing a satu-	 New England Nuclear Corporation; used as received.
rated aqueous solution of (1) by ultrafiltration of a (1)-(2) dis- persion has been described in ref 1. A Packard Tri-Carb Liquid Scintilla- tion Spectrometer was used to detect the radioactive (1) dissolved in	(2) distilled.
(2).	
	ESTIMATED ERROR:
	soly. 20% (standard deviation from 17 replicate runs).
	REFERENCES :
	 Baker, E.G. Am. Chem. Soc. Div. Petrol. Chem., Preprints- Symposia <u>1956</u>, 1, N°2, 5.

ORIGINAL MEASUREMENTS:	
Baker, E.G. <i>Science</i> <u>1959</u> , <i>129</i> , 871-4.	
PREPARED BY:	
F. Kapuku	
water at 25°C was reported	
AUXILIARY INFORMATION	
SOURCE AND PURITY OF MATERIALS:	
not specified.	

ESTIMATED ERROR:

not specified.

REFERENCES:

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