IUPAC-NIST Solubility Data Series 68. Halogenated Aliphatic Hydrocarbon Compounds C_3–C_{14} With Water

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This volume covers the solubilities of halogenated aliphatic C_3–C_{14} compounds with water, heavy water, and electrolyte solutions. All data were critically examined for their reliability and best value estimates were selected on the basis of such evaluations. Referenced works are presented in the standard IUPAC-NIST Solubility Data Series format. Reported and best value data are presented in tabular form and, where justified, data correlation equations and graphical illustrations are provided. Throughout the volume, SI conventions have been employed as the customary units. The importance of these data arises from the fact that halogenated aliphatics have considerable commercial uses in a variety of applications such as industrial chemicals, process raw materials, solvents, and the like. In such applications they are often in contact with water and are routinely exposed to the atmosphere. Sometimes such contact and exposure results from spillage, leakage, or mishandling. Reliable data are essential for concentration estimates for the halogenated aliphatics in drinking and ground water, foodstuffs, human tissue, marine organisms, and the atmosphere. The halogenated aliphatics are of particular interest to health scientists, engineers, environmentalists, and atmospheric chemists in that they represent a class of chemical materials which has many significant industrial applications. However, at the same time, some of this class of substances have been shown to be carcinogenic and also to be especially harmful for the earth's atmospheric and natural water composition. Indeed, the chemical reactivity of some halogenated aliphatics has resulted in atmospheric ozone depletion. The high ozone depletion potentials of such chemical substances emphasizes the importance of having available complete, accurate, and reliable data for mutual solubilities with water. The availability of such data is essential for estimates of halogenated aliphatic hydrocarbon levels in both natural water and aqueous industrial liquids which result from industrial fabrication, industrial liquids which result from industrial fabrication, industrial waste removal processes, and the like. The data also provide significant solubility values for studies concerning the health of humans and other biological systems. [S0047-2689(99)00403-1]

Key words: aqueous solutions; halogenated hydrocarbons; solubility.

Contents

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* Note: an asterisk (*) indicates presence of a Critical Evaluation

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1. Preface

This volume, which continues the systems provided in the substituted methanes with water and the halogenated ethanes and ethenes with water volumes of this series, contains a comprehensive collection and critical evaluation of solubility data published prior to 1993 for halogenated aliphatic C_3–C_{14} compounds with water, heavy water, seawater, and aqueous electrolyte solutions. The systems are ordered on the basis of chemical formula according to the Hill system.

A critical evaluation of the solubility data is not satisfactory without a comprehensive literature search followed by compilation of all the available information reported in journals, patents, pamphlets, brochures, books, etc. The difficulties and problems in retrieval of all solubility data are a well recognized fact. Some of the difficulties which arose during the retrieval of the original publications for this volume were:

i. The articles, reports, etc., were not cited in the Chemical Abstracts.

ii. The British Library did not hold the publications.

iii. The Slavonic Section of the British Library was unable to obtain some publications from abroad.

iv. Manufacturers' reports, leaflets, brochures, etc., were not available from industrial source.

v. University reports from experimental stations were not available from university libraries.

TABLE 1. Sources of solubility data

A. Bibliographies:
[1]J. Wisniak and A. Tamir, *Liquid-Liquid Equilibrium and Extraction. A Literature Source Book* (Elsevier, Amsterdam, 1980), 1252 pp.
[2]J. Wisniak and M. Herskowitz, *Solubility of Gases and Solids. A Literature Source Book*, Parts A and B (Elsevier, Amsterdam, 1984), p. 2070.
B. Secondary sources:
[1]G. W. Ware, *Review of Environmental Contamination and Toxicology*, Vol. 116 (Springer, New York, 1990), 200 pp.
[2]R. K. Freier, *Aqueous Solutions*, Vol. 1 (Walter de Gruyter, Berlin, 1976), 477 pp.
[3]Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, *Gleichgewichte der Absorption von Gasen in Flüssigkeiten*, Vol. 4a/c1 (Springer, Berlin, 1976), 479 pp.
[4]Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, 6th ed., Vol. 1, *Eigenschaften der Materie in Ihren Aggregationstäden*, Part 2b, *Lösungsgleichgewichte I* (Springer, Berlin, 1962).
[5]Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, 6th ed., Vol. 2, *Eigenschaften der Materie in Ihren Aggregatzustäden*, Part 2c, *Lösungsgleichgewichte II* (Springer, Berlin, 1964).
[6]A. L. Horvath, *Halogenated Hydrocarbons. Solubility-Miscibility with Water* (Marcel Dekker, New York, 1982), 889 pp.
[7]E. W. Washburn, ed. *International Critical Tables of Numerical Data*, Vol. 3 (McGraw-Hill, New York, 1928).
[8]*Beilsteins Handbuch der Organischen Chemie*, Beilstein Institut für Literatur der Organischen Chemie (Springer, Berlin, 1918–present), Vol. 1.
[9]*Kirk-Othmer Encyclopedia of Chemical Technology*, 1st, 2nd, 3rd, and 4th eds. (Wiley, New York).
[10]A. Seidell, *Solubility of Organic Compounds*, 3rd ed. (Van Nostrand, New York, 1963), 926 pp.
[11]W. F. Linke, *Solubilities of Inorganic and Metal-Organic Compounds*, 4th ed. (van Nostrand, Princeton, N.J.), Vol. 1 (1958), Vol. 2 (1965).
[12]H. Stephen and T. Stephen, *Solubilities of Inorganic and Organic Compounds*, Vols. 1 and 2 (Pergamon, Oxford, 1963).
[13]J. A. Riddich and W. B. Bunger, *Organic Solvents*, 3rd ed., Vol. 2 (Wiley-Interscience, New York, 1970), 603 pp.
[14]J. Gmeling and U. Onken, DECHEMA Data Series, *Vapor-Liquid Equilibrium Data Collection. Aqueous-Organic Systems*, Vol. 1 (1977).
[15]R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Am. Chem. Soc. Adv. in Chem. Ser. **15**, 536 pp. (1955), **22**, 491 pp. (1959), and **29**, 489 pp. (1961) (ACS, Washington, D.C.).
C. Databases:
[1]*AQUASOL Database of Aqueous Solubility*, 5th ed., S. H. Yalkowsky, ed. (University of Arizona, Tucson, Arizona, 1991).
D. Primary sources:
1. Journals
2. Reports
3. Brochures, leaflets
4. Patents
5. Private communications

TABLE 2. Conversion formulas for solubility units

a. Henry's law constant (H):

$$\text{Mass \%}\ \frac{\dfrac{P_{\text{vap}}(\text{atm})\ \ M_{\text{solute}}}{82.06\ \ T(\text{K})}}{\dfrac{H(\text{dimensionless})}{d_{\text{solvent}}}} \times 100$$

$$\text{Mass \%} = \frac{\dfrac{P_{\text{vap}}(\text{atm})\ \ M_{\text{solute}}}{H\ \ (\text{m}^3\ \text{atm/mol})}}{d_{\text{solvent}}} \times 10^{-4}$$

$$H\ \ (\text{dimensionless}) = \frac{C_{\text{air}}}{C_{\text{solvent}}} = \frac{16.04 P_{\text{vap}}(\text{atm})\ \ M_{\text{solute}}}{T(\text{K})\ \ S_{\text{solute}}(\text{mg/dm}^3)}$$

b. Air/water partition coefficient (K_{AW}):

$$\text{Mass \%} = \frac{100\ \ K_{\text{AW}} P_{\text{vap}}}{82.054\ \ T(\text{K})\ \ d_{\text{solvent}}}$$

c. Distribution ratio (p/c):

$$(p/c) = \frac{\text{solute vapor pressure}}{\text{solute concentration}}\ \frac{(\text{mm Hg})}{(\text{mmole/dm}^3)}$$

d. Partition coefficient (K):

$$K = \frac{1}{\text{Ostwald coefficient}} = \frac{1}{L}$$

e. Distribution coefficient (K_i):

$$K_i = \text{Ostwald coefficient}\ \ L = \frac{Y_i}{x_i}$$

In summary, there were several cases where the original sources were not obtainable and the information had to be taken from secondary sources.

The referenced literature sources can be classified into the following groups:

A. Bibliographies
B. Secondary sources (books, reviews)
C. Databases (computer softwares)
D. Primary sources (journals, reports, etc.)

A list of the various sources of solubility data following the above classification is summarized in Table 2.

Once a copy of the original document—usually a photocopy—was obtained, the first step was to read it carefully. Often the original article was in a foreign language which required a translation. If the description was not focused on the solubility aspect, then often some relevant details, e.g., source and purity of the solute and solvent, or both, were not included in the text. In many cases, the method, apparatus, and procedure were simply referred to other articles. Furthermore, when the experimental errors were not stated, the compiler sometimes introduced a subjective judgement for the accuracy of the measured solubility and temperature. The estimated accuracy of the measured quantities is quite subjective and the readers must take this fact into consideration.

The summaries of the procedures and abstracts were based on the available description of the method, apparatus, and procedures. Often a short statement ''Details are not available,'' had to be used when the main contents of the articles focused not on solubility measurements but some other aspects of chemistry.

The conversion of the published solubility data into conventional units often presented difficulties, particularly when the dimensions were not expressed clearly. For example, the Henry's law constants, separation coefficients, distribution ratio, partition coefficients, etc., were not specified explicitly. Some of the more relevant conversion formulas are given in Table 3.

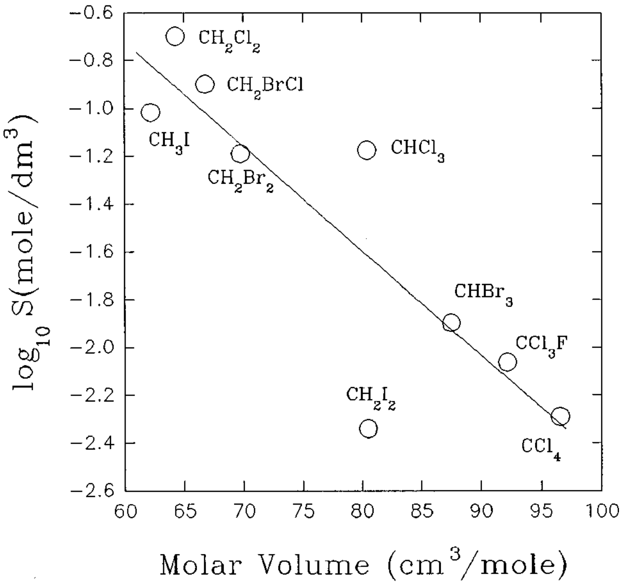

FIG. 1. Logarithm of saturated molarity vs solute molar volume at 25 °C for halogenated methanes in water.

To convert solubility data from one unit to another, often the density and vapor pressure of the pure components and/or of the mixture were needed. The physical properties of the pure compounds were taken from the DIPPR[1] and TRCVP[2] databases. To find or derive the physical properties of mixtures required a more elaborate effort. Experimental data, e.g., density and vapor pressure for aqueous solutions of halogenated hydrocarbons are extremely rare in the literature. Consequently, approximations were obtained using calculations recommended in standard handbooks, e.g., Reid *et al.*[3] An illustration of the difficulty of obtaining accurate conversions is shown by the following typical case.

The solubility of carbon tetrachloride (CCl_4) in water (H_2O) is 0.10 $\mathrm{cm^3/100\,cm^3}$ water at 25 °C. The solubility in mass percent ($\mathrm{g\,CCl_4/100\,g\,soln.}$) is required. The density of pure carbon tetrachloride is $1.5834\,\mathrm{g\,CCl_4/cm^3}$ at 25 °C (DIPPR database). The solution density is required to convert the pure water density using the mass of the aqueous solution of carbon tetrachloride at 25 °C. However, the density of the aqueous solution of carbon tetrachloride has not been reported in the literature. The reason is quite simple; the difference between the density of pure water and that of the aqueous solution of carbon tetrachloride at 25 °C is marginal. As a consequence, the errors obtained upon the determination of solubility are considerably greater than the possible difference between the solubility in pure water or in its aqueous solutions at the same temperature. It follows, in this case, one must use the approximation

$$\mathrm{g\,CCl_4/100\ g\ H_2O} \approx \mathrm{g\,CCl_4/100\ g\ soln.}$$

On the other hand, for solubility values larger than, say, 2–3 mass percent, the differences become significant, as the following example illustrates. The solubility in water of dichloromethane (CH_2Cl_2) is 2.363 g/100 g water at 0 °C. The solubility in $\mathrm{g\,CH_2Cl_2/100\,g\,soln.}$ at the same temperature is required. If 100 g water dissolves $2.363\,\mathrm{g\,CH_2Cl_2}$, then the total mass of the solution becomes 102.363 g. This means that 100 g aqueous solution will dissolve less CH_2Cl_2 than 100 g pure water, that is,

$$\frac{2.363\ \mathrm{g\,CH_2Cl_2}}{102.363\ \mathrm{g\,soln.}}100=2.3084\ (\mathrm{g\ \ CH_2Cl_2/100\ \ g\,soln.}).$$

The result is $2.3084\,\mathrm{g\,CH_2Cl_2/100\,g\,soln.}$ at 0 °C. Consequently, there is a 2.31% reduction in the solubility relative to 100 g pure water. This is in comparison to the reduction of only 0.10% in the case of the solubility of CCl_4 in 100 g water or 100 g aqueous solution at 25 °C.

All critical evaluations of the solubility data are presented on the evaluation sheets. The information available on the relevant compilation sheets served as the fundamental source for the critical evaluations. The following main aspects of the solubility data have been considered:

Purity of the components (solute and solvents)
Date of the experiment
Accuracy of the method
Reproducibility of the experiment
Experience of the investigator(s), previous publications
Consistency of the data, trends in series.

Once these aspects of the works had been examined, efforts were made to weight the reliability of the reported data. As much as possible, the differences in the quality of the data have been taken into account.

The available solubility data for binary systems may be very scarce, medial, or abundant, depending on the commercial application of the systems. Whenever data from different sources exist, they often disagree. For evaluation of the agreement or disagreement among the data, graphical presentations usually provide the clearest picture. The figures normally contain the original data from all references for a given system. A plot representing the solubility data (expressed in mole fraction or mass percent) can reveal whether or not a trend exists among the data in addition to highlighting any discrepancies of the experimental solubility measurements.

The final data can be classified as:

obscure or dubious—rejected data
tentative—not recommended data
recommended—good agreement among the published results.

A graphical presentation of the solubility data may be performed on linear, semilogarithmic, etc., scales. The unit of solubility may be given as specific or molar scales. For practical reasons, the mass percent unit is often used, whereas the mole fraction is another common unit of solubility. In this volume most figures are plotted using one of two different scales. For the solubilities in water, linear graphs are used and for the solubilities of water in halogenated hydrocarbons, the so called Cox chart is applied. In the Cox charts, the solubility of water is given as $\log_{10} x_2$ vs $1/T$. A straight line on a Cox plot can be very useful for revealing consistent data covering a limited temperature range. However, the straight line does not apply for solubility data over a very wide temperature interval, e.g., from the triple point to the critical point. Therefore, in some cases (e.g., some of the polyhalogenated ethanes with water solubilities), the normal polynomial equations were used for smoothing the solubility data.

To fit experimental data into the various equations, the individual data points are often weighted. The smoothed data may be influenced somewhat by such procedures of weighting individual data points. Data analysis is a process of mathematical and/or graphical treatment of experimental data through the use of statistical or parametric procedures. Whenever the raw data are fragmentary, the aim is to generate an extended range of internally consistent values by synthesis. In any case, the temperature dependence of solubility must be examined and any unusual irregularities must be investigated carefully.

The temperature dependence of the solubility of halogenated hydrocarbons in water has been correlated using normal polynomial equations over limited temperature intervals. These equations should be used only in the temperature range indicated. The equations play two major roles; to provide data users with interpolated data with good accuracy and to provide data users with acceptable data for use in computer programs, if desired. The deviation of the various experimental values from the fitted data are given as standard or average deviations.

If the experimental data cover a reasonable temperature interval, then the data and the smoothing equation are often illustrated in a figure. The graphical presentation of the reported and fitted data clearly indicates the risks involved when one attempts to extrapolate the raw experimental data. In some cases, an extrapolation is quite safe for the desired temperature (see for example, the solubility of water in halogenated hydrocarbons in moderate temperature intervals); whereas, in other cases, the risk is very high and it is not recommended. The shape of the solubility curves suggests the extrapolation and interpolation possibilities.

Whether the mutual solubility between two liquids is partial or complete depends on the similarities or differences between the molecules of the two chemical compounds. The halogenated hydrocarbon and water systems are only partially miscible without exception. Furthermore, the miscibility or immiscibility of water with other liquids is also very dependent upon temperature. At ambient temperature and atmospheric pressure, the miscibility is very limited between water and halogenated hydrocarbons. For most systems, the mutual solubility is less than 2 mass percent.

In a liquid–liquid system the variation of solubility with temperature depends on the sign of the heat of mixing or solution. The minimum dissolution temperature occurs for most halogenated hydrocarbon–water systems between 270 and 310 K. The interactions between the solute and solvent molecules provide the explanation for the phenomena. The temperature dependence of solubility is a result of temperature dependent structural modifications of water. A different energy is required for cavity formation and for the changes in rigidity of the lattice as temperature is changed.

The appearance of these minima resembles the dependence of the critical micelle concentration upon temperature. Here, the iceberg formation of water molecules around the monodisperse solute enhances the critical micelle concentration, the logarithm of which would be decreased linearly with $1/T$ provided the solution behaves regularly, and the iceberg formation increases with a temperature reduction.

It is well recognized that the rare gases and hydrocarbon gases form iceberg-like structures when dissolved in cold water, followed by an iceberg melting as the temperature is raised. The solubility of most gases in water shows a minimum when plotted against temperature. The shape of the solubility curves for molecules with alkyl groups is explained by considering that the ice-like structure of water is also formed around the nonpolar alkyl group of molecules in water. This structure tends to break down as the temperature of the solution is increased.

The minimum solubility temperature can be calculated from a calorimetric measurement of the enthalpy of solution at infinite dilution $(\Delta_{\text{soln}}H^{\infty})$. This value is very large and varies from negative to positive values within a small temperature range. Consequently, very large errors may be caused by an erroneous interpretation. In addition to the enthalpy of solution, the change in the heat capacity at infinite dilute aqueous solution $(\Delta_{\text{soln}}C_p^{\infty})$ is required for the calculation of the minimum solubility temperature (T_{min});

$$T_{\text{min}}=298.15\ \text{K}-\frac{\Delta_{\text{soln}}H^{\infty}(298.15\ \text{K})}{\Delta_{\text{soln}}C_p^{\infty}}.$$

A more detailed description of the minimum solubility phenomenon is given by Horvath,[4] Shinoda,[5] Nishino and Nakamura,[6] and Privalov and Gill.[7]

The relations between the solubility and some of the physical properties of the solute or solvent have been investigated from early times in solution studies. The various experiments showed that in very diluted solutions the influence of the solute molecules does not extend to all solvent molecules in the solution. Consequently, the large fraction of solvent molecules, which are not affected by solute molecules, must exist more or less in the same state of aggregation as in the pure state. A change of solvent molar volume in dilute solutions is very small. However, in more concentrated solutions the effects of the presence of the solute molecules on the solvent molecules are not negligible. The amount of molar volume change of the solvent depends on the nature of the solutes. The dissolution process is related to the disintegration of the solute in the solvent, as compared to its pure state molecular order, as a result of the mutual action of attraction of the solute and solvent.

In general, solubility depends on many parameters and is of a very complex nature. There is no simple relation established between solubility and the other properties of the pure components (solute and solvent). Despite the lack of a simple relationship, the solubility of halogenated benzenes in water at 25 °C has been correlated with a reasonable success using the molar volume of the solutes.[8] Similarly, the solubility of halogenated methanes in water shows a linear relationship.[9] The correlation is based on the assumption that the molar volumes in saturated solutions are not greatly different from those in the pure state. The simple linear relation at 25 °C is illustrated graphically in Fig. 1. This is a very useful and practical way to show the consistency of the solubility data. Any significant deviation from such a linear relationship suggests some inconsistency and introduces doubt concerning the reliability of the data.

Correlation equation:

$$\log(S/\text{mole/dm}^3) = 1.8995 - 4.3707 \times 10^{-2} \; (V_m/\text{cm}^3\,\text{mole}^{-1}).$$

1.1. References

[1] DIPPR, *Design Institute for Physical Property Data* (Am. Inst. Chem. Eng., New York, 1985), Software package for IBM PC.

[2] TRCVP, *Thermodynamic Research Center* (Texas A & M University System, College Station, TX, 1989).

[3] R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids*, 4th ed. (McGraw-Hill, New York, 1987), 742 pp.

[4] A. L. Horvath, *Halogenated Hydrocarbons: Solubility-Miscibility with Water* (Marcel Dekker, New York, 1982), 889 pp.

[5] K. Shinoda, J. Phys. Chem. **81**, 1300 (1977).

[6] N. Nishino and M. Nakamura, Bull. Chem. Soc. Jpn. **51**, 1617 (1978).

[7] P. L. Pivalo and S. J. Gill, Pure Appl. Chem. **61**, 1097 (1989).

[8] A. L. Horvath and F. W. Getzen, *Halogenated Benzenes, Toluenes and Phenols With Water*, IUPAC Solubility Data Series, Vol. 20 (Pergamon, Oxford, 1985), 266 pp.

[9] S. Horiba, *Memories of the College of Science and Engineering* (Kyoto Imperial University, 1917), Vol. 2, p. 1-43.

2. Introduction to the Solubility Data Series. Solubility of Liquids in Liquids

2.1. Nature of the Project

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids, and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

This series is concerned primarily with liquid–liquid systems, but a limited number of related solid–liquid, fluid–fluid, and multicomponent (organic–water–salt) systems are included where it is considered logical and appropriate. Solubilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

2.2. Compilations and Evaluations

The formats for the compilations and critical evaluations have been standardized for all volumes. A description of these formats follows.

2.2.1. Compilations

The format used for the compilations is, for the most part, self-explanatory. A compilation sheet is divided into boxes, with detailed contents described below.

Components: Each component is listed according to IUPAC name, formula, and Chemical Abstracts (CA) Registry Number. The Chemical Abstracts name is also included if this differs from the IUPAC name, as are trivial names if appropriate. IUPAC and common names are cross-referenced to Chemical Abstracts names in the System Index.

The formula is given either in terms of the IUPAC or Hill[1] system and the choice of formula is governed by what is usual for most current users: i.e., IUPAC for inorganic compounds, and Hill system for organic compounds. Components are ordered on a given compilation sheet according to:

(a) saturating components;
(b) nonsaturating components in alphanumerical order;
(c) solvents in alphanumerical order.

The saturating components are arranged in order according to the IUPAC 18-column periodic table with two additional rows:

Columns 1 and 2:	H, alkali elements, ammonium, alkaline earth elements
Columns 3 to 12:	transition elements
Columns 13 to 17:	boron, carbon, nitrogen groups; chalcogenides, halogens
Column 18:	noble gases
Row 1:	Ce to Lu
Row 2:	Th to the end of the known elements, in order of atomic number.

Organic compounds within each Hill formula are ordered in the following succession:

(a) by degree of unsaturation;
(b) by order of increasing chain length in the parent hydrocarbon;
(c) by order of increasing chain length of hydrocarbon branches;
(d) numerically by position of unsaturation;
(e) numerically by position by substitution;
(f) alphabetically by IUPAC name.

Example:

C_5H_8	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C_5H_{10}	cyclopentane
	3-methyl-1-butene
	2-methyl-2-butene
	1-pentene
	2-pentene

TABLE 3. Interconversions between quantities used as measures of solubilities: c-component systems containing c-1 solutes i and single solvent c

	x_i	w_i	m_i	c_i
$x_i=$	x_i	$\dfrac{1}{1+\dfrac{M_i}{M_c}\left\{\dfrac{1}{w_i}-1+\sum_{j\neq 1}^{c-1}\left(\dfrac{M_c}{M_f}-1\right)\dfrac{w_j}{w_i}\right\}}$	$\dfrac{1}{1+\dfrac{1}{m_iM_c}+\sum_{j\neq i}^{c-1}\dfrac{m_j}{m_i}}$	$\dfrac{1}{1+\dfrac{1}{M_c}\left(\dfrac{\rho}{c_i}-M_i\right)+\sum_{j\neq i}^{c-1}\dfrac{c_j}{c_i}\left(1-\dfrac{M_j}{M_c}\right)}$
$w_i=$	$\dfrac{1}{1+\dfrac{M_c}{M_i}\left\{\dfrac{1}{x_i}-1+\sum_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right\}}$	w_i	$\dfrac{1}{1+\dfrac{1}{m_iM_i}\left(1+\sum_{j\neq i}^{c-1}m_jM_j\right)}$	$\dfrac{c_iM_i}{\rho}$
$m_i=$	$\dfrac{1}{M_c\left(\dfrac{1}{x_i}-1-\sum_{j\neq i}^{c-1}\dfrac{x_j}{x_i}\right)}$	$\dfrac{1}{M_i\left(\dfrac{1}{w_i}-1-\sum_{j\neq i}^{c-1}\dfrac{w_j}{w_i}\right)}$	m_i	$\dfrac{1}{\dfrac{1}{c_i}\left(\rho-\sum_{j\neq i}^{c-1}c_jM_j\right)-M_i}$
$c_i=$	$\dfrac{\rho}{M_i+M_c\left\{\dfrac{1}{x_i}-1+\sum_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right\}}$	$\dfrac{\rho w_i}{M_i}$	$\dfrac{\rho}{\dfrac{1}{m_i}\left(1+\sum_{j\neq i}^{c-1}m_jM_j\right)+M_j}$	c_i

ρ: density of solution; M_i : molar masses of i. For relations for two-component systems, set summations to 0.

C_5H_{12}	2,2-dimethylpropane
	2-methylbutane
	pentane
$C_5H_{12}O$	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
$C_6H_{12}O$	cyclohexanol
	4-methyl-1-penten-3-ol
	1-hexen-3-ol
	4-hexen-3-ol

Deuterated (^{2}H) compounds follow immediately the corresponding H compounds.

Original Measurements: References are abbreviated in the forms given by Chemical Abstracts Service Source Index (CASSI). Names originally in other than Roman alphabets are given as transliterated by Chemical Abstracts. In the case of multiple entries (for example, translations) an asterisk indicates the publication used for compilation of the data.

Variables: Ranges of temperature, pressure, etc., are indicated here.

Prepared by: The names of all compilers are given here.

Experimental Values: Components are described as (1), (2), etc., as defined in the ‘‘Components’’ box. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; e.g., mass percent for weight percent; mol dm^{-3} for molar; etc. In most cases, both mass and molar values are given. Usually, only one type of value (e.g., mass percent) is found in the original paper, and the compiler has added the other type of value (e.g., mole percent) from computer calculations based on 1989 atomic weights.[2] Temperatures are expressed as t/°C, t/°F or T/K as in the original; if necessary, conversions to T/K are made, sometimes in the compilations, and always in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations[3] as far as possible.

Errors in calculations, fitting equations, etc., are noted, and where possible corrected. Material inserted by the compiler is identified by the word ‘‘compiler’’ or by the compiler's name in parentheses or in a footnote. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper, conversions from concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

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

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

Method: The apparatus and procedure are mentioned briefly. Abbreviations used in Chemical Abstracts are often used here to save space, reference being made to sources of further detail if these are cited in the original paper.

Source and Purity of Materials: For each component, referred to as (1), (2), etc., the following information (in this order and in abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity.

Estimated Error: If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by ‘‘compiler’’ or the compiler’s name in parentheses or in a footnote) from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on Ku and Eisenhart.[4]

Comments and/or Additional Data: Many compilations include this section which provides short comments relevant to the general nature of the work or additional experimental and thermodynamic data which are judged by the compiler to be of value to the reader.

References: The format for these follows the format for the Original Measurements box, except that final page numbers are omitted. References (usually cited in the original paper) are given where relevant to interpretation of the compiled data, or where cross-reference can be made to other compilations.

2.2.2. Evaluations

The evaluator’s task is to assess the reliability and quality of the data, to estimate errors where necessary, and to recommend ‘‘best’’ values. The evaluation takes the form of a summary in which all the data supplied by the compiler have been critically reviewed. There are only three boxes on a typical evaluation sheet, and these are described below.

Components: The format is the same as on the Compilation sheets.

Evaluator: The name and affiliation of the evaluator(s) and date up to which the literature was checked.

Critical Evaluation:

(a) Critical text. The evaluator checks that the compiled data are correct, assesses their reliability and quality, estimates errors where necessary, and recommends numerical values based on all the published data (including theses, reports and patents) for each given system. Thus, the evaluator reviews the merits or shortcomings of the various data. Only published data are considered. Documented rejection of some published data may occur at this stage, and the corresponding compilations may be removed.

The solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. Although many systems have been studied by at least two workers, the range of temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature, although both sets of results were obtained by reliable methods. In such cases, a definitive assessment may not be possible. In some cases, two or more sets of data have been classified as tentative even though the sets are mutually inconsistent.

(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 on all the compilation sheets, stating the limits within which it should be used.

(c) Graphical summary. In addition to (b) above, graphical summaries are often given.

(d) Recommended values. Data are recommended if the results of at least two independent groups are available and they are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the applied experimental and computational procedures. Data are reported as tentative if only one set of measurements is available, or if the evaluator considers some aspect of the computational or experimental method as mildly undesirable but estimates that it should cause only minor errors. Data are considered as doubtful if the evaluator considers some aspect of the computational or experimental method as undesirable but still considers the data to have some value where the order of magnitude of the solubility is needed. Data determined by an inadequate method or under ill-defined conditions are rejected. However, references to these data are included in the evaluation together with a comment by the evaluator as to the reason for their rejection.

(e) References. All pertinent references are given here, including all those publications appearing in the accompanying compilation sheets and those which, by virtue of their poor precision, have been rejected and not compiled.

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units[3] when the data can be converted accurately.

2.3. Quantities and Units Used in Compilation and Evaluation of Solubility Data

2.3.1. Mixtures, Solutions, and Solubilities

A *mixture*[5,6] describes a gaseous, liquid, or solid phase containing more than one substance, where the substances are all treated in the same way.

A *solution*[5,6] describes a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent*, and may itself be a mixture, is treated differently than the other substances, which are called *solutes*. If the sum of the mole fractions of the solutes is small compared to unity, the solution is called a *dilute solution*.

The *solubility* of a solute 1 (solid, liquid, or gas) is the analytical composition of a saturated solution, expressed in terms of the proportion of the designated solute in a designated solvent.[7]

‘‘Saturated’’ implies equilibrium with respect to the processes of dissolution and demixing; the equilibrium may be stable or metastable. The solubility of a substance in metastable equilibrium is usually greater than that of the same substance in stable equilibrium. (Strictly speaking, it is the activity of the substance in metastable equilibrium that is greater.) Care must be taken to distinguish true metastability from supersaturation, where equilibrium does not exist.

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients, and osmotic coefficients. Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components.

2.3.2. Physicochemical Quantities and Units

Solubilities of solids have been the subject of research for a long time, and have been expressed in a great many ways, as described below. In each case, specification of the temperature and either partial or total pressure of the saturating gaseous component is necessary. The nomenclature and units follow, where possible, Ref. 3. A few quantities follow the ISO standards[8] or the German standard,[9] see a review by Cvitas[10] for details.

A note on nomenclature. The nomenclature of the IUPAC *Green Book*[3] calls the solute component B and the solvent component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the *Green Book*.

1. *Mole fraction* of substance 1, x_1 or $x(1)$:

$$x_1=\frac{n_1}{\sum_{s=1}^{c} n_s}, \tag{1}$$

where n_s is the amount of substance of *s*, and *c* is the number of distinct substances present (often the number of thermodynamic components in the system). *Mole percent* of substance 1 is $100x_1$.

2. *Ionic mole fractions* of salt *I*, x_{i+}, x_{i-}:
For a mixture of *s* binary salts *i*, each of which ionizes completely into ν_{s+} cations and ν_{s-} anions, with $\nu_s=\nu_{s+}+\nu_{s-}$ and a mixture of *p* nonelectrolytes *j*, of which some may be solvent components, a generalization of the definition in Ref. 11 gives:

$$x_{i+}=\frac{\nu_{i+}x_i}{1+\sum_{i=1}^{s}(\nu_i-1)x_s}, \quad x_{i-}=\frac{\nu_{i-}x_{i+}}{\nu_{i+}} \quad i=1...s, \tag{2}$$

$$x'_j=\frac{x_j}{1+\sum_{i=1}^{s}(\nu_i-1)x_i}, \quad j=(s+1),\ldots,p. \tag{3}$$

The sum of these mole fractions is unity, so that, with $c=s+p$,

$$\sum_{i=1}^{s}(x_{i+}+x_{i-})+\sum_{i=s+1}^{c}x'_i=1. \tag{4}$$

General conversions to other units in multicomponent systems are complicated. For a three-component system containing nonelectrolyte 1, electrolyte 2, and solvent 3,

$$x_1=\frac{\nu_{2+}x'_1}{\nu_{2+}-(\nu_2-1)x_{2+}}, \quad x_2=\frac{x_{2+}}{\nu_{2+}-(\nu_2-1)x_{2+}}. \tag{5}$$

These relations are used in solubility equations for salts, and for tabulation of salt effects on solubilities of gases (see below).

3. *Mass fraction* of substance 1, w_1 or $w(1)$:

$$w_1=\frac{g_1}{\sum_{s=1}^{c} g_s}, \tag{6}$$

where g_s is the mass of substance *s*. *Mass percent* of substance 1 is $100w(1)$ or $100w_1$. The equivalent terms *weight fraction, weight percent*, and *g(1)/100g solution* are no longer used.

4. *Molality* of solute 1 in a solvent 2, m_1:

$$m_1=\frac{n_1}{n_2M_2} \tag{7}$$

SI base units: mol kg^{-1}. Here, M_2 is the molar mass of the solvent.

5. *Aquamolality, Solvomolality* of substance 1 in a mixed solvent with components 2, 3,[12] $m_1^{(3)}$:

$$m_1^{(3)}=\frac{m_1\bar{M}}{M_3} \tag{8}$$

SI base units: mol kg^{-1}. Here, the average molar mass of the solvent is

$$\bar{M}=x'_2M_2+(1-x'_2)M_3, \tag{9}$$

and x'_2 is the solvent mole fraction of component 2. This term is used most frequently in discussing comparative solubilities in water (component 2) and heavy water (component 3) and in their mixtures.

6. *Amount concentration* of solute 1 in a solution of volume *V*, c_1:

$$c_1=(\text{formula of solute})=n_1/V \tag{10}$$

SI base units: mol m^{-3}. The symbol c_1 is preferred to [formula of solute], but both are used. The old terms *molarity, molar*, and *moles per unit volume* are no longer used.

7. *Mass concentration* of solute 1 in a solution of volume *V*, r_1: SI base units: kg m^{-3}.

$$\rho_1=g_1/V \tag{11}$$

8. *Mole ratio*, $r_{\mathrm{A,B}}$ (dimensionless) (10)

$$r_{\mathrm{A,B}}=n_1/n_2 \tag{12}$$

Mass ratio, symbol $\zeta_{\mathrm{A,B}}$, may be defined analogously.[10]

Mole 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. Conversions between pairs of these quantities can be carried out using the equations given in Table 1 at the end of this Introduction. Other useful quantities will be defined in the prefaces to individual volumes or on specific data sheets.

9. *Density*, ρ:

$$\rho=g/V \tag{13}$$

SI base units: kg m^{-3}. Here *g* is the total mass of the system.

10. *Relative density*, $d=\rho/\rho°$: the ratio of the density of a mixture at temperature *t*, pressure *p* to the density of a ref-

erence substance at temperature t', pressure p'. For liquid solutions, the reference substance is often water at 4 °C, 1 bar. (In some cases 1 atm is used instead of 1 bar.) The term *specific gravity* is no longer used.

Thermodynamics of Solubility

Thermodynamic analysis of solubility phenomena provides a rational basis for the construction of functions to represent solubility data, and thus aids in evaluation, and sometimes enables thermodynamic quantities to be extracted. Both these are often difficult to achieve because of a lack of experimental or theoretical activity coefficients. Where thermodynamic quantities can be found, they are not evaluated critically, since this task would involve examination of a large body of data that is not directly relevant to solubility. Where possible, procedures for evaluation are based on established thermodynamic methods. Specific procedures used in a particular volume will be described in the Preface to that volume.

2.4. References for the Introduction

[1] E. A. Hill, J. Am. Chem. Soc. **22**, 478 (1990).

[2] IUPAC Commission on Atomic Weights and Isotopic Abundances, Pure Appl. Chem. **63**, 975 (1989).

[3] I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry* (the *Green Book*). (Blackwell Scientific, Oxford, UK, 1993).

[4] H. H. Ku, p. 73; C. Eisenhart, p. 69; in H. H. Ku, ed., *Precision Measurement and Calibration*, NBS Special Publication 300, Vol. 1 (NBS, Washington, 1969).

[5] J. Regaudy and S. P. Klesney, *Nomenclature of Organic Chemistry (IUPAC)*, (the *Blue Book*), (Pergamon, Oxford, 1979).

[6] V. Gold *et al.*, eds., *Compendium of Chemical Technology* (the *Gold Book*) (Blackwell Scientific, Oxford, UK, 1987).

[7] H. Freisen and G. H. Nancollas, eds., *Compendium of Analytical Nomenclature* (the *Orange Book*). (Blackwell Scientific, Oxford, UK, 1987). Sect. 9.1.8.

[8] ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).

[9] German Standard, DIN 1310, *Zusammungsetzung von Mischphasen* (Beuth, Berlin, 1984).

[10] T. Cvitaš, Chem. Int. **17**, 123 (1995).

[11] R. A. Robinson and R. H. Stokes, *Electrolyte Solutions*, 2nd ed. (Butterworths, London, 1959).

[12] J. W. Lorimer, in *Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems)*, edited by R. Cohen-Adad and J. W. Lorimer, IUPAC Solubility Data Series, Vol. 47 (Pergamon, Oxford, UK, 1991), p. 495.

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3. Halogenated Aliphatic Compounds C_3–C_{14} Solubilities

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane; $C_3Br_2F_6$; [661-95-0]; R-216B2

Original Measurements:

du Pont de Nemours & Company, Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, Wilmington, Del., 17 pp. (1966).

Variables:

T/K=294

Prepared By:

A. L. Horvath

4. 1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane with Water

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
21	6.8×10^{-3}	1.17	3.77×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane; $C_3Cl_2F_6$; [661-97-2]; R-216

Original Measurements:

du Pont de Nemours & Company, Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, Wilmington, Del., 17 pp. (1966).

Variables:

T/K=294

Prepared By:

A. L. Horvath

5. 1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane with Water

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
21	9.6×10^{-3}	1.18	5.33×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,1-Trichloro-2,2,3,3,3-pentafluoropropane; $C_3Cl_3F_5$; [4259-43-2]; R-215

Original Measurements:

du Pont de Nemours & Company, Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, Wilmington, Del., 17 pp. (1966).

Variables:

T/K=294

Prepared By:

A. L. Horvath

6. 1,1,1-Trichloro-2,2,3,3,3-pentafluoropropane with Water

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$ mol g^{-1} (compiler)
21	5.8×10^{-3}	7.64	3.22×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,1,3-Tetrachloro-2,2,3,3-tetrafluoropropane; $C_3Cl_4F_4$; [2268-46-4]; R-214

Original Measurements:

du Pont de Nemours & Company, Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, Wilmington, Del., 17 pp. (1966)

Variables:

T/K=294

Prepared By:

A. L. Horvath

7. 1,1,1,3-Tetrachloro-2,2,3,3-tetrafluopropane with Water

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$ mol g^{-1} (compiler)
21	5.2×10^{-3}	7.32	2.89×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	Evaluator:
(1) 1,1,2,3,3,3-Hexachloro-1-propene; Cl_3Cl_6; [1888-71-7] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

8. 1,1,2,3,3,3-Hexachloro-1-propene with Water

Critical Evaluation

The 1,1,2,3,3,3-hexachloropropene (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2,3,3,3-hexachloropropylene (1) in water (2) and part 2 is water (2) in 1,1,2,3,3,3-hexachloropropene (1).

Part 1. The solubility of 1,1,2,3,3,3-hexachloropropene (1) in water (2) has been studied by three work groups in the temperature range from 288 to 313 K. The data of Dreisbach[1] and of Simonov *et al.*[2] were reported at only a single temperature, that is, at 298.15 and 313.15 K, respectively. The temperature dependence of solubility was measured by Antropov *et al.*[3] in the narrow temperature interval between 288.15 and 299.15 K.

The data are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be prescribed. All reported experimental solubility values in mass percent and mole fraction are summarized in Table 4.

TABLE 4. Reported solubility of 1,1,2,3,3,-hexachloropropene (1) in water (2)

Temperature		Solubility		Reference
°C	K	100 w_1	10^6 x_1	
15	288.15	9.47×10^{-4}	0.686	3
20	293.15	1.18×10^{-3}	0.855	3
25	298.15	15.0×10^{-3}	10.9	1
26	299.15	1.70×10^{-3}	1.231	3
40	313.15	5.00×10^{-3}	3.62	2

Part 2. The solubility of water (2) in 1,1,2,3,3,3-hexachloropropene (1) between 288 and 323 K has been measured by five groups of researchers. The measured solubility of Dreisbach[1] is markedly higher than all other studies and is therefore rejected. The remaining solubility data originated from workers of the same organization over a number of years.[2–5] The solubility data were reported at different temperatures, except for the value at 299.15 K. The data are in good agreement and they were used for the smoothing equation of mole fraction solubility of water in 1,1,2,3,3,3-hexachloropropene between 288 and 323 K:

$$\log_{10} x_2 = 2.2310 - 1604.19/(T/\mathrm{K}).$$

This equation, representing the combined data, yielded a standard deviation of 2.38×10^{-2}. The linear relation between the solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature is illustrated in Fig. 2. The straight line behavior of such plots is characteristic of the solubility of water in halogenated hydrocarbons, as discussed in the Preface.

The tentative solubility values at 5 K intervals for water (2) in 1,1,2,3,3,3-hexachloropropene (1) in weight percent and mole fraction are presented in Table 5.

TABLE 5. Tentative solubility of water (2) in 1,1,2,3,3,3-hexachloropropene (1)

Temperature		Solubility	
°C	K	100 w_2	10^4 x_2
15	288.15	3.51×10^{-3}	4.61
20	293.15	4.37×10^{-3}	5.74
25	298.15	5.40×10^{-3}	7.09
30	303.15	6.62×10^{-3}	8.69
35	308.15	8.07×10^{-3}	10.60
40	313.15	9.77×10^{-3}	12.83
45	318.15	1.18×10^{-2}	15.44
50	323.15	1.41×10^{-2}	18.48

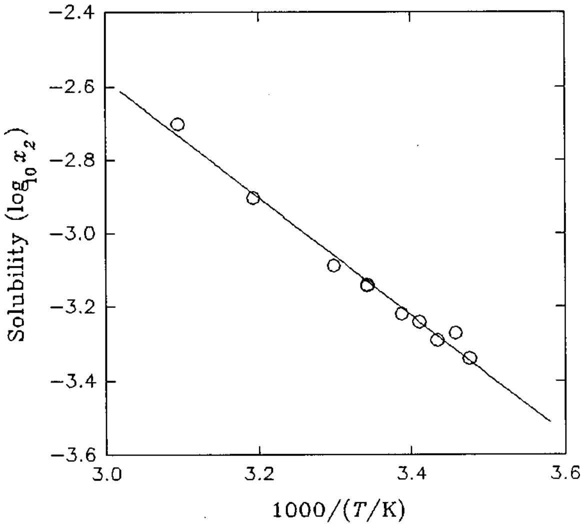

FIG. 2. Solubility of water (2) in 1,1,2,3,3,3-hexachloropropene (1).

References:

[1] R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. 22 (Am. Chem. Soc., Washington, D.C., 1959), p. 412.

[2] V. D. Simonov, V. E. Pogulyai, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **44**, 1755 (1970).

[3] L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.

[4] V. D. Simonov *et al.*, Dokl. Neftekim. Sekt. Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 346 (1971).

[5] V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).

Components:	**Original Measurements:**
(1) 1,1,2,3,3-Hexachloro-1-propene; C_3Cl_6; [1888-71-7] (2) Water; H_2O; [7732-18-5]	R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. 22 (Am. Chem. Soc., Washington, D.C., 1959), p. 412

Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^5\ x_1$ (compiler)	100 g_2/g_1	$10^3\ x_2$ (compiler)
25	1.5×10^{-2}	1.09	1.4×10^{-2}	1.93

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemical Co., purified by distillation before use. The f.p. was −57.12 °C.
(2) Distilled

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,1,2,3,3,3-Hexachloro-1-propene; C_3Cl_6; [1888-71-7]	V. D. Simonov, V. E. Pogulyai, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **44**, 1755 (1970).

Variables:	**Prepared By:**
T/K=303–323	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	$10\ w_1 M_1^{-1}$/mol g^{-1} (compiler)
30	5.90×10^{-3}	8.14	3.27×10^{-4}
50	1.44×10^{-2}	19.85	7.99×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of water and 1,1,2,3,3,-hexachloro-1-propene was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Synthesized by the authors and further purified by distillation.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,3,3,3-Hexachloro-1-propene; C_3Cl_6; [1888-71-7]

Original Measurements:

V. D. Simonov *et al.*, Dokl. Neftekim. Sekt. Bashkir. Respub. Prav. Vses. Khim. Obshchest. 346-51 (1971).

Variables:

T/K=288–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^5\ w_1$ Alekseev	$10^5\ w_1$ Fischer	$10^5\ w_1$ Spectroscopy	$10^4\ x_1$ (compiler) Alekseev	$10^4\ x_1$ (compiler) Fischer	$10^4\ x_1$ (compiler) Spectroscopy
14.5	3.35	3.32	3.30	4.624	4.582	4.555
16	3.93	3.89	3.85	5.424	5.369	5.313
20	4.07	—	4.24	5.619	—	5.865
26	5.25	5.20	5.30	7.244	7.175	7.313

Auxiliary Information

Method/Apparatus/Procedure:

The determination of the solubility of water in 1,1,2,3,3,3-hexachloro-1-propene was based on the infrared spectroscopic method. A UR-20 spectrophotometer was used with 2 cm cuvettes and the windows made of KBr. The spectra were recorded at 3600–810 cm^{-1}, and the absorbance at 3702 cm^{-1} was found by the baseline method. Standard mixtures of 1,1,2,3,3,3-hexachloro-1-propene and water were used for the calibration graphs. The results obtained were compared with the measurements made by the methods of cloud point[1] and a Karl Fischer titration.

Source and Purity of Materials:

(1) Distilled.
(2) Synthesized by the authors, distilled, washed with $HClSO_3$ and water and again distilled. Finally dried with $CaCl_2$ and P_2O_5.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

References:

[1] V. F. Alekseev, Wied. Ann. **28**, 305 (1886).

Components:

(1) 1,1,2,3,3,3-Hexachloro-1-propene; C_3Cl_6; [1888-71-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.

Variables:

T/K=288–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^7\ x_1$ (compiler)	100 w_2	$10^4\ x_2$ (compiler)
15	9.47×10^{-4}	6.86	—	—
18	—	—	3.71×10^{-3}	5.12
20	11.8×10^{-4}	8.55	—	—
22	—	—	4.38×10^{-3}	6.04
26	17.0×10^{-4}	12.31	5.25×10^{-3}	7.24

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of water and 1,1,2,3,3,3-hexachloro-1-propene was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Synthesized by the investigators, purified by fractional distillation and dried with $CaCl_2$ and P_2O_5.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:	**Original Measurements:**
(1) 1,1,2,3,3,3-Hexachloro-1-propene; C_3Cl_6; [1888-71-7] (2) Water; H_2O; [7732-18-5]	V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).
Variables:	**Prepared By:**
T/K=313	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^6 x_1 (compiler)	10 w_2	10^3 x_2 (compiler)
40	5.0×10^{-3}	3.62	9.1×10^{-3}	1.25

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alexejew was used. Further details are found elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

References:
[1] V. D. Simonov, L. N. Popova, T. M. Shamsutdinov, V. E. Pogulyai, and F. A. Mamina, Symp. Doklady Neftekhimicheskoi Sektsii, Ufa. No. 6 (1971).

Components:	**Original Measurements:**
(1) 3-Chloro-1,1,1-trifluoropropane; $C_3H_4ClF_3$; [460-35-5] (2) Water; H_2O; [7732-18-5]	G. V. Selyuzhitskii, Prom. Zagryazmeniya Vodoemov 112 (1967).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

9. 3-Chloro-1,1,1-trifluoropropane with Water

Experimental Data

t/°C	ρ_1 /kg m^{-3}	10^4 x_1 (compiler)	100 w_1 (compiler)
20	1.33	1.81	0.133

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,2-Dichloro-1-propene; $C_3H_4Cl_2$; [563-54-2] (2) Water; H_2O; [7732-18-5]	B. G. Chitwood, Advances Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

10. 1,2-Dichloro-1-propene with Water

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.27	4.39	2.43×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [542-75-6] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

11. 1,3-Dichloro-1-propene with Water

Critical Evaluation

The solubility of 1,3-dichloro-1-propene (1) in water (2) has been studied by three work groups; whereas, the solubility of water (2) in 1,3-dichloro-1-propene (1) has not been investigated yet.

The solubility data of 1,3-dichloro-1-propene (1) in water (2) are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be assigned. All the available data for the solubility of 1,3-dichloro-1-propene (1) in water (2) in mass percent and mole fraction are summarized in Table 6.

TABLE 6. Reported solubility of 1,3-dichloro-1-propene (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^4\ x_1$	Reference
25	298.15	0.03	0.487	1
24.85	298.00	0.103	1.68	2
20	293.15	0.451	7.35	3
30	303.15	0.429	6.99	3
40	313.15	0.420	6.85	3

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).
[2] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
[3] C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience, New York, 1962), pp. 47–84.

Components:

(1) 1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [542-75-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Adv. Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	3.0×10^{-2}	4.87	2.70×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [542-75-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. P. Warner, J. M. Cohen, and J. C. Ireland, Determination of Henry's Law Constants of Selected Priority Pollutants, U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July, 1987).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
24.85	3.55×10^{-3}	0.1032	1.676

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants are described elsewhere.[1] The general procedure was to add an excess quantity of 1,3-dichloro-1-propene to distilled de-ionized water, place the sample in a thermostat bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. 1,3-Dichloro-1-propene was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from a log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used without further purification. Stated purity was >99%.
(2) Distilled de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W.-Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) 1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [542-75-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	100 w_1 (compiler)	10^4 x_1 (compiler)
20	1360±30	0.451	7.35
30	1430±25	0.429	6.99
40	1460±85	0.420	6.85

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,3-dichloro-1-propene (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. 1,3-Dichloro-1-propene was injected into the mixture cells and a magnetic stirrer was turned on. Then, the cells were allowed to equilibrate. The stirrer was then turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered, and de-ionized.

Estimated Errors:

Solubility: See above.
Temperature: ±0.05 K.

Components:

(1) cis-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-01-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

12. cis-1,2-Dichloro-1-propene with Water

Critical Evaluation

The solubility of cis-1,3-dichloro-1-propene (1) in water (2) has been studied by two work groups; whereas, the solubility of water (2) in cis-1,3-dichloro-1-propene (1) has not been investigated yet.

The solubility of cis-1,3-dichloro-1-propene (1) in water (2) at 30 °C has been measured by McNally and Grob and the results have been reported in two papers.[1,2] Despite the similar method, apparatus, and procedures, the reported data are in very poor agreement. The datum of Goring[3] is significantly higher than those of McNally and Grob.[1,3] In the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be proposed. All the available data for the solubility of cis-1,3-dichloro-1-propene (1) in water (2) in mass percent and mole fraction are summarized in Table 7.

TABLE 7. Reported solubility of cis-1,3-dichloro-1-propene (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
20	293.15	2.69×10^{-1}	4.38	3
30	303.15	1.07×10^{-1}	1.74	1
30	303.15	9.14×10^{-2}	1.49	2

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).
[2] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
[3] C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience, New York, 1962), pp. 47–84.

Components:

(1) cis-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-01-5]
(2) Water H_2O; [7732-18-5]

Original Measurements:

C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience, New York, 1962), pp. 47–84.

Variables:

$T/K=293$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	2.70×10^3	0.269	4.38

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The experimental work was done in the Main Analytical Laboratory, The Dow Chemical Company, Midland, Michigan. Further details have been reported elsewhere.[1]

Source and Purity of Materials:

(1) Dow Chemical Company, Midland, Michigan. Used as received.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] C. R. Youngson and C. A. Goring, Soil Sci. **93**, 306 (1962).

Components:

(1) cis-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-01-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Variables:

$T/K=303$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	1.071×10^3	0.1070	1.739

Auxiliary Information

Method/Apparatus/Procedure:

Standard solutions were prepared in 100 cm^3 flask. They were shaken for 5 min and then allowed to equilibrate in a constant temperature bath held at 30 °C for 24 h. Samples were pipetted in headspace vials, sealed, thermostated and then examined by the gas chromatographic head space analysis technique. An F & M model 402 gas chromatograph, equipped with dual columns and dual flame ionization detectors, was used.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±93.7 ppm std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) cis-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-01-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	9.112×10^2	9.143×10^{-2}	1.485

Auxiliary Information

Method/Apparatus/Procedure:

Standard cis-1,3-dichloro-1-propene solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±8.72% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:

(1) trans-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-02-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

13. trans-1,3-Dichloro-1-propene with Water

Critical Evaluation

The solubility of trans-1,3-dichloro-1-propene (1) in water (2) has been studied by two work groups, whereas the solubility of water (2) in trans-1,3-dichloro-1-propene (1) has not been investigated yet.

The solubility of trans-1,3-dichloro-1-propene (1) in water (2) at 30 °C has been determined by McNally and Grob and their results have been reported in two papers.[1,2] Despite similar methods, apparatus, and procedures, the reported data are in poor agreement. The value of Goring[3] is markedly higher than the measurements of McNally and Grob.[1,2] In the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be suggested. All the available data for the solubility of trans-1,3-dichloro-1-propene (1) in water (2) in mass percent and mole fraction are summarized in Table 8.

TABLE 8. Reported solubility of trans-1,3-dichloro-1-propene (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
20	293.15	0.279	4.54	3
30	303.15	0.119	1.93	1
30	303.15	0.102	1.66	2

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).
[2] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
[3] C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience, New York, 1962), pp. 47–84.

Components:	**Original Measurements:**
(1) trans-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-02-6] (2) Water; H_2O; [7732-18-5]	C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience New York, 1962), pp. 47–84.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	2.80×10^3	0.279	4.54

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The experimental work was done in the Main Analytical Laboratory, The Dow Chemical Company, Midland, Michigan. Further details have been reported elsewhere.[1]

Source and Purity of Materials:

(1) Dow Chemical Company, Midland, Michigan. Used as received.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] C. R. Youngson and C. A. Goring, Soil Sci. **93**, 306 (1962).

Components:	**Original Measurements:**
(1) trans-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-02-6] (2) Water; H_2O; [7732-18-5]	M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).
Variables:	**Prepared By:**
T/K=303	A. L. Horvath

Experimental Data

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	1.1881×10^3	0.1187	1.929

Auxiliary Information

Method/Apparatus/Procedure:

Standard solutions were prepared in 100 cm^3 flask. They were shaken for 5 min and then allowed to equilibrate in a constant temperature bath held at 30 °C for 24 h. Samples were pipetted in headspace vials, sealed, thermostated and then examined by the gas chromatographic head space analysis technique. An F & M model 402 gas chromatograph, equipped with dual columns and dual flame ionization detectors, was used.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±126.8 ppm std. dev.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) trans-1,3-Dichloro-1-propene; $C_3H_4Cl_2$; [10061-02-6] (2) Water; H_2O; [7732-18-5]	M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
Variables:	**Prepared By:**
T/K=303	A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	1.0199×10^3	0.1023	1.662

Auxiliary Information

Method/Apparatus/Procedure:

Standard trans-1,3-dichloro-1-propene solutions of increasing concentration were prepared in volumetic flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.

(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±10.7% std. dev.

Temperature: ±0.5 K (compiler)

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:	**Original Measurements:**
(1) 2,3-Dichloro-1-propene; $C_3H_4Cl_2$; [78-88-6] (2) Water; H_2O; [7732-18-5]	G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).
Variables:	**Prepared By:**
T/K=291	A. L. Horvath

14. 2,3-Dichloro-1-propene with Water

Experimental Data

Water origin	$g_1V_2^{-1}$/kg m^{-3} (compiler)	100 w_1	10^4 x_1 (compiler)
De-ionized water	2.75±0.05	0.275	4.475
Artificial seawater	1.847±0.008	0.1847	—
Mediterranean seawater	1.70±0.2	0.170	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 2,3-dichloro-1-propene was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.

(2) Source and purity of water, artificial and Mediterranean seawaters not given.

Estimated Errors:

Solubility: See above.

Temperature: ±1 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, G. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **11**, 178 (1983).

Components:

(1) 3-Bromo-1-propene; C_3H_5Br; [106-95-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

15. 3-Bromo-1-propene with Water

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	3.17×10^{-2}	0.382	5.71

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 3-bromo-1-propene. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a high pressure liquid chromatographic procedure, which has been described elsewhere.[1] The result is an average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K

References:

[1] H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. **86**, 361 (1981).

Components:

(1) 3-Bromo-1-propene; C_3H_5Br; [106-95-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	31.7	0.383	5.72

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 3-bromo-1-propene. The saturated solution was then pumped through an extractor column and 3-bromo-1-propylene was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both an ultraviolet (UV) absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:
(1) 1,2-Dibromo-3-chloropropane; $C_3H_5Br_2Cl$; [96-12-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. A. I. Goring, in *Advances in Pest Control Research*, edited by R. L. Metcalf (Interscience, New York, 1962), pp. 47–84.

Variables:
T/K=298

Prepared By:
A. L. Horvath

16. 1,2-Dibromo-3-chloropropane with Water

Experimental Data

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	1.23×10^3	0.123	3.387

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The experimental work was done in the Main Analytical Laboratory, The Dow Chemical Company, Midland, Michigan. Further details have been reported elsewhere.[1]

Source and Purity of Materials:

(1) Dow Chemical Company, Midland, Michigan. Used as received.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±1 K (compiler).

References:
[1] C. R. Youngson and C. A. I. Goring, Soil Sci. **93**, 306 (1962).

Components:
(1) 3-Chloro-1-propene; C_3H_5Cl; [107-05-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Yu. A. Treger, R. M. Flid, and S. S. Spektor, Russ. J. Phys. Chem. **38**, 253 (1964).

Variables:
T/K=298–343

Prepared By:
A. L. Horvath

17. 3-Chloro-1-propene with Water

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	4.0	3.98×10^{-1}	9.40
50	1.3	1.30×10^{-1}	3.06
70	0.82	8.20×10^{-2}	1.93

Auxiliary Information

Method/Apparatus/Procedure:

Nitrogen was saturated with 3-chloro-1-propene vapor and bubbled through a thermostatically controlled cell filled with a known volume of water. The saturation condition was achieved after 2–3 h. The saturated solution was sampled periodically and analyzed by colorimetry. Duplicate samples were taken at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: ±2%.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) 3-Chloro-1-propene; C_3H_5Cl; [107-05-1] (2) Hydrogen chloride; HCl; [7647-01-0] (3) Water; H_2O; [7732-18-5]	Yu. A. Treger, R. M. Flid, and S. S. Spektor, Russ. J. Phys. Chem. **38**, 253 (1964).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

18. 3-Chloro-1-propene with Hydrogen Chloride and Water

Experimental Data

wt. % HCl	t/°C	$10^3\ g_1/g_3$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
5	25	0.90	8.83×10^{-2}	2.13
	50	0.85	8.40×10^{-2}	2.03
	70	1.09	10.89×10^{-2}	2.63
10	25	0.96	9.20×10^{-2}	2.28
	50	1.24	11.97×10^{-2}	3.14
	70	1.38	13.46×10^{-2}	3.34
15	25	1.02	9.54×10^{-2}	2.43
	50	1.50	14.14×10^{-2}	3.61
	70	1.95	18.51×10^{-2}	4.72
20	25	1.25	11.42×10^{-2}	2.99
	50	1.92	17.74×10^{-2}	4.65

Auxiliary Information

Method/Apparatus/Procedure:

Nitrogen was saturated with 3-chloro-1-propene vapor and bubbled through a thermostatically controlled cell filled with a known volume and concentration of hydrochloric acid solution. The saturation condition was achieved after 2–3 h. The saturated solution was sampled periodically and analyzed by colorimetry. Duplicate samples were taken at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler).

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.05 K.

Components:	**Evaluator:**
(1) 1,2,3-Trichloropropane; $C_3H_5Cl_3$; [96-18-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

19. 1,2,3-Trichloropropane with Water

Critical Evaluation

The solubility of 1,2,3-trichloropropane (1) in water (2) has been studied by four work groups, whereas the solubility of water (2) in 1,2,3-trichloropropane (1) has not been investigated yet.

The solubility value of Wright and Schaffer[1] is markedly higher than the other measurements and is therefore rejected. The remaining data of Hutchinson *et al.*,[2] of Leighton and Calo,[3] and of Bauduin *et al.*[4] are in reasonable agreement, although further studies are required before any values can be recommended.

The combined mass percent data[2–4] covering the temperature interval from 275 to 298 K were correlated to obtain the following mass percent (1) equation:

$$\text{solubility}\ [100\ w_1] = -14.676 + 0.097\ 906(T/\text{K}) - 1.610\ 15\times10^{-4}(T/\text{K})^2,$$

which yielded a standard deviation of 1.47×10^{-2} in the prescribed temperature range. The concave shape of the solubility versus temperature curve suggests that the data may be inconsistent. The tentative solubility at 5 K intervals from the smoothing equation for this system in mass percent and mole fraction are presented in Table 9.

TABLE 9. Tentative solubility of 1,2,3-trichloropropane (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^4\ x_1$
5	278.15	9.92×10^{-2}	1.21
10	283.15	1.37×10^{-1}	1.68
15	288.15	1.67×10^{-1}	2.04
20	293.15	1.88×10^{-1}	2.30
25	298.15	2.01×10^{-1}	2.47

References:

[1] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

[2] T. C. Hutchinson *et al.*, *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–586.

[3] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

[4] G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Components:

(1) 1,2,3-Trichloropropane; $C_3H_5Cl_3$; [96-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$V_2g_1^{-1}/m^3\ g^{-1}$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	4.20×10^{-4}	0.238	2.91

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,2,3-trichloropropane with a large volume of water and then measuring the volume of the undissolved portion of 12,2,3-trichloropropane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2,3-Trichloropropane; $C_3H_5Cl_3$; [96-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

T. C. Hutchinson *et al.*, *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–586.

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$\rho_1\ /kg\ m^{-3}$	$10^4\ x_1$ (compiler)	$100\ w_1$ (compiler)
25	1.900	2.33	0.1906

Auxiliary Information

Method/Apparatus/Procedure:

An excess quantity of 1,2,3-trichloropropane was added to water and stirred vigorously for 24 h. After settling at 25 °C for 48 h, the solution was extracted with cyclohexane. The samples were analyzed using an Aminco–Bowman spectrophotofluorometer. A detailed description of the method has been reported elsewhere.[1]

Source and Purity of Materials:

(1) Aldrich Chemicals, highest grade available. Used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.2 K (compiler).

References:

[1] D. Mackay and W.-Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Components:	**Original Measurements:**
(1) 1,2,3-Trichloropropane; $C_3H_5Cl_3$; [96-18-4] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=275–298	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
1.9	11.66	7.230×10^{-2}	0.8841
13.5	11.46	1.651×10^{-1}	2.021
15.7	13.55	1.596×10^{-1}	1.953
17.1	14.18	1.683×10^{-1}	2.060
22.0	15.12	2.173×10^{-1}	2.661
24.9	19.81	2.000×10^{-1}	2.448

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

5 μL 1,2,3-trichloropropane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,2,3-trichloropropane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±6.1%.
Temperature: ±0.5 K

Components:	**Original Measurements:**
(1) 1,2,3-Trichloropropane; $C_3H_5Cl_3$; [96-18-4] (2) Water; H_2O; [7732-18-5]	G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).
Variables:	**Prepared By:**
T/K=291	A. L. Horvath

Experimental Data

Water origin	$g_1 V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
De-ionized water	1.75±0.01	0.175	2.142
Artificial seawater	1.70±0.02	0.170	—
Mediterranean seawater	1.39±0.09	0.139	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,2,3-trichloropropane was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity of the de-ionized water and artificial and Mediterranean seawaters not given.

Estimated Errors:

Solubility: See above.
Temperature: ±1 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, G. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **11**, 178 (1983).

Components:	**Evaluator:**
(1) 1-Bromo-3-chloropropane; C_3H_6BrCl; [109-70-6] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

20. 1-Bromo-3-chloropropane with Water

Critical Evaluation

The solubility of 1-bromo-3-chloropropane (1) in water (2) has been studied by three work groups; whereas, the solubility of water (2) in 1-bromo-3-chloropropane (1) has not been investigated yet.

The solubility value of Dreisbach[1] at 25 °C is greater by a factor of 8.1 than those of Tewari *et al.*[2] and of Miller *et al.*[3] The data reported in the latter two papers originate from the same laboratory and the agreement is therefore sound. Not enough workers have measured the solubility of 1-bromo-3-chloropropane in water over common ranges of temperature to provide recommended solubility values. Further studies will be necessary before even tentative values can be prescribed. All the available data for the solubility of 1-bromo-3-chloropropane (1) in water (2) in mass percent and mole fraction are summarized in Table 10.

TABLE 10. Reported solubility of 1-bromo-3-chloropropane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
25	298.15	1.807	21.4	1
25	298.15	0.223	2.56	2
25	298.15	0.224	2.56	3

References:

[1] R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. **22** (Am. Chem. Soc., Washington, D.C., 1959), p. 212.

[2] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[3] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromo-3-chloropropane; C_3H_6BrCl; [109-70-6] (2) Water; H_2O; [7732-18-5]	R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. **22** (Am. Chem. Soc., Washington, D. C., 1959), p. 212.
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.84	1.807	2.14

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemical Company, 99.79% pure, purified by distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) 1-Bromo-3-chloropropane; C_3H_6BrCl; [109-70-6] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	1.42×10^{-2}	0.223	2.56

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromo-3-chloropropane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1-Bromo-3-chloropropane; C_3H_6BrCl; [109-70-6] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.42×10^{1}	0.224	2.56

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromo-3-chloropropane. The saturated solution was then pumped through an extractor column and 1-bromo-3-chloropropane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both an UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dibromopropane; $C_3H_6Br_2$; [78-75-1]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

21. 1,2-Dibromopropane with Water

Critical Evaluation

The 1,2-dibromopropane (1) and water (2) binary system is treated in two parts; part 1 is 1,2-dibromopropane (1) in water (2) and part 2 is water (2) in 1,2-dibromopropane (1).

Part 1. The solubility of 1,2-dibromopropane (1) in water (2) has been studied by two work groups at two different temperatures. Therefore, a comparison of the measured values is not possible. The readers are referred to the relevant compilation sheets of Dreisbach[1] and of Bauduin *et al.*,[2] respectively.

Part 2. The solubility of water (2) in 1,2-dibromopropane (1) has been studied by Dreisbach[1] only and there are no other measurements for comparison. Therefore, it is not possible to perform a critical evaluation. The readers are referred to the relevant compilation sheet for further details.

References:

[1] R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. **22** (Am. Chem. Soc., Washington, D.C., 1959), p. 214.

[2] G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Components:

(1) 1,2-Dibromopropane; $C_3H_6Br_2$; [78-75-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. 22 (Am. Chem. Soc., Washington, D.C., 1959), p. 214.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^4\ x_1$ (compiler)	100 g_2/g_1	$10^3\ x_2$ (compiler)
25	0.143	1.28	5.2×10^{-2}	5.80

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemical Company, 99.86% pure, purified by distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,2-Dibromopropane; $C_3H_6Br_2$; [78-75-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Variables:

T/K=291

Prepared By:

A. L. Horvath

Experimental Data

Water origin	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
De-ionized water	0.82±0.03	8.20×10^{-2}	7.23
Artificial seawater	0.801±0.003	8.01×10^{-2}	—
Mediterranean seawater	0.82±0.05	8.20×10^{-2}	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,2-dibromopropane was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.

Estimated Errors:

Solubility: See above.
Temperature: ±1 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, G. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **11**, 178 (1983).

Components:

(1) 1,3-Dibromopropane; $C_3H_6Br_2$; [109-64-8]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

22. 1,3-Dibromopropane with Water

Critical Evaluation

The 1,3-dibromopropane (1) and water (2) binary system is treated in two parts; part 1 is 1,3-dibromopropane (1) in water (2) and part 2 is water (2) in 1,3-dibromopropane (1).

Part 1. The solubility of 1,3-dibromopropane (1) in water (2) has been studied by three work groups in the narrow temperature range from 298.15 to 303.15 K. Within the narrow temperature range for the solubility data of Gross and Saylor,[1] of Chitwood,[2] and of Mackay *et al.*,[3] the agreement is very good. In the absence of other independent studies, it is not possible to say whether or not the solubility behavior between 298.15 and 303.15 K should increase or decrease with increasing temperature. Further studies will be necessary before the slope of the solubility curve can be established. All the available data for the solubility of 1,3-dibromopropane (1) in water (2) in mass percent and mole fraction are summarized in Table 11.

TABLE 11. Tentative solubility of 1,3-dibromopropane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
30	303.15	1.68×10^{-1}	1.50	1
25	298.15	1.70×10^{-1}	1.52	2
25	298.15	1.69×10^{-1}	1.52	3

Part 2. The solubility of water (2) in 1,3-dibromopropane (1) has been studied only by Mackay *et al.*[3] and there are no other measurements for comparison. Therefore, it is not possible to perform a critical evaluation. The readers are referred to the relevant compilation sheet for further details.

References:

[1] P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).
[2] B. G. Chitwood, Advances in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).
[3] D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U.S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

Components:
(1) 1,3-Dibromopropane; $C_3H_6Br_2$; [109-64-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).

Variables:
T/K=303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	1.68	0.168	1.50

Auxiliary Information

Method/Apparatus/Procedure:
The saturated solution was prepared in a flask and placed in a waterbath thermostat. The samples were analyzed using a Zeiss combination liquid and gas interferometer described elsewhere.[1] A detailed description of the complete procedure is given in a M. A. thesis.[2]

Source and Purity of Materials:
(1) Eastman Kodak Company, fractionally distilled before use. The b. p. range was 166.64–166.86 °C.
(2) Distilled.

Estimated Errors:
Solubility: ±0.5%.
Temperature: ±0.02 K.

References:
[1] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[2] M. A. Gorman, MA thesis, Duke University, Durham, 1932.

Components:
(1) 1,3-Dibromopropane; $C_3H_6Br_2$; [109-64-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. G. Chitwood, Advances in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^4\ x_1$ (compiler)	$10\ w_1 M_1^{-1}$/mol g^{-1}
25	0.17	1.52	8.42×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,3-Dibromopropane; $C_3H_6Br_2$; [109-64-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U.S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)	100 w_2 (compiler)	10^3 x_2
25	8.4	0.17	1.52	1.8×10^{-2}	2.0

Auxiliary Information

Method/Apparatus/Procedure:

An aqueous solution with an excess amount of 1,3-dibromopropane was stirred for 1 day before being introduced into a 1 L glass vessel. Nitrogen entered at the bottom of the vessel through a sintered glass disk. The exit gas flow rate was measured by a soap bubble flow meter. The concentration of 1,3-dibromopropane in water was determined by gas chromatography (GC). The GC was equipped with both a dual flame ionization detector and an electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Doubly distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1.0 K.

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

23. 1,2-Dichloropropane with Water

Critical Evaluation

The 1,2-dichloropropane (1) and water (2) binary system is treated in two parts; part 1 is 1,2-dichloropropane (1) in water (2) and part 2 is water (2) in 1,2-dichloropropane (1).

Part 1. The solubility of 1,2-dichloropropane (1) in water (2) has been studied by 15 work groups in the temperature range from 275 to 313 K. The data of Chiou *et al.*[1] are markedly higher than the solubility values calculated from the smoothing equation and are therefore rejected. The measurements of McNally and Grob[2,3] and of Howe *et al.*[4] are significantly lower than other solubility data and are also rejected.

The remaining data from eleven laboratories were compiled or used for the smoothing equation. The combined measurements of Gross,[5] of Wright and Schaffer,[6] of McClure,[7] of McGovers,[8] of Chitwood,[9] of Dreisbach,[10] of Sato and Nakijima,[11] of Leighton and Calo,[12] of Mackay *et al.*,[13] of Warner *et al.*,[14] and of Wright *et al.*[15] were correlated to obtain the following mass percent (1) equation:

$$\text{solubility }[100\,w_1]=3.3285-0.021\,464(T/\text{K})+3.7632\times10^{-5}(T/\text{K})^2,$$

which yielded a standard deviation of 8.56×10^{-3} in the temperature range from 275 to 313 K. The curve obtained from the smoothing equation shows a distinct minimum of 285.18 K as shown in Fig. 3.

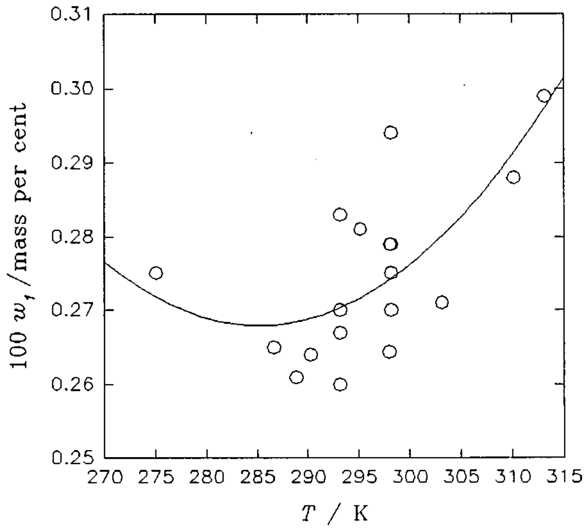

FIG. 3. Solubility of 1,2-dichloropropane (1) in water (2).

The recommended solubility values at 5 K intervals for 1,2-dichloropropane in water in weight percent and mole fraction are presented in Table 12.

TABLE 12. Recommended solubility of 1,2-dichloropropane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
5	278.15	270×10^{-1}	4.31
10	283.15	2.68×10^{-1}	4.28
15	288.15	2.68×10^{-1}	4.28
20	293.15	2.70×10^{-1}	4.31
25	298.15	2.74×10^{-1}	4.38
30	303.15	2.80×10^{-1}	4.48
35	308.15	2.88×10^{-1}	4.60
40	313.15	2.97×10^{-1}	4.75

Part 2. The solubility of water (2) in 1,2-dichloropropane (1) has been reported in five sources covering the narrow temperature range from 293 to 298 K. The data are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be prescribed. All the available data for the solubility of water (2) in 1,2-dichloropropane (1) in mass percent and mole fraction are summarized in Table 13.

TABLE 13. Reported solubility of water (2) in 1,2-dichloropropane (1)

Temperature		Solubility		
°C	K	100 w_2	10^3 x_2	Reference
20	293.15	7.0×10^{-2}	4.37	7
25	298.15	11.68×10^{-2}	7.28	16
20	293.15	4.0×10^{-2}	2.50	8
25	298.15	13.2×10^{-2}	8.22	10
25	298.15	3.19×10^{-2}	2.00	13

References:

[1] C. T. Chiou and V. H. Freed, Chemodynamic Studies on Bench Mark Industrial Chemicals, U.S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

[2] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

[3] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

[4] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida, 86 pp. (September, 1987); AD-A188 571.

[5] P. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

[6] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

[7] H. B. McClure, Ind. Eng. Chem., News Ed. **17**, 149 (1939).

[8] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[9] B. G. Chitwood, Advances in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

[10] R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. 22 (Am. Chem. Soc., Washington, D.C., 1959), p. 211.

[11] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

[12] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

[13] D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U.S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

[14] H. P. Warner, J. M. Cohen, and J. C. Ireland, Determination of Henry's Law Constants of Selected Priority Pollutants, U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July, 1987).

[15] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

[16] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Components:	**Original Measurements:**
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5] (2) Water; H_2O; [7732-18-5]	P. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.280	0.279	4.45

Auxiliary Information

Method/Apparatus/Procedure:

A weighted amount of 1,2-dichloropropane was mixed with 1000 g water in a bottle and immersed in a water thermostat bath. The bottle was placed on a shaker and shaken until no more liquid droplets remained undissolved. The concentration of the 1,2-dichloropropane in water was determined by a Zeiss water interferometer. One or more samples were syphoned out for the solubility determination. The German translation also has been published.[1]

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K

References:

[1] P. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	3.40×10^2	0.294	4.70

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,2-dichloropropane with a large volume of water and measuring the volume of the undissolved portion.

Source and Purity of Materials:

(1) Commercial reagent, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. B. McClure, Ind. Eng. Chem. News Ed. **17**, 149 (1939).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	10^4 x_1 (compiler)	100 g_2/g_1	10^3 x_2 (compiler)
20	0.26	4.15	7.0×10^{-2}	4.37

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) Water; H_2O; [7732-18-5]
(2) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]

Original Measurements:
C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1M^{-1}/mol g^{-1}	$10^3\ x_1$ (compiler)	100 w_1 (compiler)
25	6.481×10^{-3}	7.280	0.1168

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of water and 1,2-dichloropropane was introduced into an equilibration flask and then lowered into the waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:
(1) Distilled.
(2) Source not given. Purity and dried before use.

Estimated Errors:
Solubility: $\pm7\times10^{-6}$ avg. dev.
Temperature: ±0.05 K.

References:

[1] M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey, eds., *Production of Heavy Water* (McGraw-Hill, New York, 1955), p. 129.

Components:
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
20	0.27	4.31	4.0×10^{-2}	2.50

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:
(1) Commercial grade. Source not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Advances in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:

$T/\text{K}=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\text{C}$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1 M_1^{-1}/\text{mol g}^{-1}$ (compiler)
25	0.27	4.31	2.39×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. R. Dreisbach, *Physical Properties of Chemical Compounds*, Adv. in Chem. Ser. No. 22 (Am. Chem. Soc., Washington, D.C., 1959), p. 211.

Variables:

$T/\text{K}=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\text{C}$	$100\ g_1/g_2$	$10^4\ x_1$ (compiler)	$100\ g_1/g_2$	$10^3\ x_2$ (compiler)
25	0.275	4.39	0.132	8.22

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemical Company, 99.76% pure, purified by distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, Chemodynamic Studies on Bench Mark Industrial Chemicals, U. S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
3	3.71	0.370	5.92
20	3.57	0.356	5.69
34	3.75	0.376	6.01

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g 1,2-dichloropropane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on the determination and evaluation procedures are found elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou, and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp. 1980, pp. 28–42 (Publ. 1981).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Water/air coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	5.4	0.288	4.60

[a] Gas–liquid partition parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

1,2-Dichloropropane vapor was equilibrated in an airtight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.1 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=275–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
1.9	45.8	0.275	4.39
13.5	90.2	0.265	4.23
15.7	101.6	0.261	4.17
17.1	108.6	0.264	4.22
22.0	131.4	0.281	4.49
24.9	153.5	0.279	4.46

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,2-dichloropropane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,2-dichloropropane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.0%.
Temperature: ±0.5 K.

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U. S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

Variables:

T/K=293–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)	100 w_2 (compiler)	10^3 x_2
20	25.0	0.283	4.51	—	—
25	—	—	—	3.19×10^{-2}	2.0

Auxiliary Information

Method/Apparatus/Procedure:

An aqueous solution with an excess amount of 1,2-dichloropropane was stirred for 1 day before being introduced into a 1 L glass vessel. Nitrogen entered at the bottom of the vessel through a sintered glass disk. The exit gas flow rate was measured by a soap bubble flow meter. The concentration of 1,2-dichloropropane in water was determined by gas chromatography. The GC was equipped with both a dual flame ionization detector and an electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Doubly distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1.0 K.

Components:
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. E. McNally and R. L. Grob. J. Chromatogr. **260**, 23 (1983).

Variables:
T/K=303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	2.4204×10^3	0.2415	3.858

Auxiliary Information

Method/Apparatus/Procedure:
Standard solutions were prepared in a 100 cm^3 flask. They were shaken for 5 min and then allowed to equilibrate in a constant temperature bath held at 30 °C for 24 h. Samples were pipetted in headspace vials, sealed, thermostated and then examined by the gas chromatographic head space analysis technique. An F & M model 402 gas chromatograph, equipped with dual columns and dual flame ionization detectors, was used.

Source and Purity of Materials:
(1) Chemical Service, West Chester, PA., USA, purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:
Solubility: ±10.36% rel. err.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:
T/K=303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	ρ_1 /g m^{-3}	$10^4\ x_1$ (compiler)	$100\ w_1$ (compiler)
30	2.069×10^3	3.373	0.2074

Auxiliary Information

Method/Apparatus/Procedure:
Standard 1,2-dichloropropane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:
(1) Chemical Service, West Chester, PA., USA, purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:
Solubility: ±5.89% std. dev.
Temperature: ±0.5 K (compiler).

References:
[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, (1983).

Components:	Original Measurements:
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5] (2) Water; H_2O; [7732-18-5]	H. P. Warner, J. M. Cohen, and J. C. Ireland, Determination of Henry's Law Constants of Selected Priority Pollutants, U. S. EPA Technical Report PB87-212684, Cincinnati, OH (July, 1987).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	2.82×10^{-3}	0.2644	4.225

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants are described elsewhere.[1] The general procedure was to add an excess quantity of 1,2-dichloropropane to distilled de-ionized water, place the sample in a thermostat bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. 1,2-Dichloropropane was stripped isothermally from the solution at a know gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, stated purity >99%, used as received.
(2) Distilled de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W.-Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:	Original Measurements:
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida, 86 pp. (September, 1987); AD-A188 571.
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	10^6 w_1	100 w_1 (compiler)	10^4 x_1 (compiler)
10	2.062×10^3	0.2062	3.294
20	2.030×10^3	0.2030	3.242
30	1.867×10^3	0.1867	2.982

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled de-ionized water and sealed. Measured volumes of the 1,2-dichloropropane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a free induction decay (FID) detector. The GC responses were compared with calibration plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure. Used as received.
(2) Distilled de-ionized.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	100 w_1 (compiler)	10^4 x_1 (compiler)
20	2340±30	0.267	4.27
30	2310±30	0.271	4.33
40	2090±30	0.299	4.78

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,2-dichloropropane (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. 1,2-Dichloropropane was injected into the mixture cells and a magnetic stirrer was turned on. Then, the cells were allowed to equilibrate. The stirrer was then turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2)Distilled, filtered, and de-ionized.

Estimated Errors:

Solubility: See above.
Temperature: ±0.05 K.

Components:

(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]
(2) Magnesium sulfate; $MgSO_4$; [7587-88-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

T/K=298
Concentration(2)/mol dm^{-3}=0.5

Prepared By:

A. L. Horvath

24. 1,2-Dichloropropane with Magnesium Sulfate and Water

Experimental Data

t/°C	c_2 /mol dm^{-3}	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.50	0.160	0.160	2.693

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10–20 cm^3 1,2-dichloropropane in 500 cm^3 of an aqueous $MgSO_4$ solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,2-dichloropropane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractinally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K.

Components:	**Original Measurements:**
(1) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5] (2) Potassium chloride; KCl; [3811-04-9] (3) Water; H_2O; [7732-18-5]	P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).
Variables:	**Prepared By:**
T/K=298 Concentration(2)/mol dm^{-3}=0.5	A. L. Horvath

25. 1,2-Dichloropropane with Potassium Chloride and Water

Experimental Data

t/°C	c_2 /mol dm^{-3}	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.50	0.241	0.2.40	3.046

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10–20 cm^3 1,2-dichloropropane in 500 cm^3 of an aqueous KCl solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,2-dichloropropane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K.

Components:	**Original Measurements:**
(1) Water-d_2; D_2O; [7789-20-0] (2) 1,2-Dichloropropane; $C_3H_6Cl_2$; [78-87-5]	C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

26. 1,2-Dichloropropane with Water-d_2

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	5.218×10^{-3}	0.1045	5.866

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and 1,2-dichloropropane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: $\pm6\times10^{-6}$ avg. dev.
Temperature: ±0.05 K.

References:

[1] M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey, eds., *Production of Heavy Water* (McGraw-Hill, New York, 1955), p. 129.

Components:	**Evaluator:**
(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

27. 1,3-Dichloropropane with Water

Critical Evaluation

The solubility of 1,3-dichloropropane (1) in water (2) has been studied by six work groups; whereas, the solubility of water (2) in 1,3-dichloropropane (1) has not been investigated yet.

All the data of six laboratories were compiled or used for the smoothing equation. The combined data points of Gross,[1] of Wright and Schaffer,[2] of Gross *et al.*,[3] of Chitwood,[4] of Leighton and Calo,[5] and of Bauduin *et al.*[6] were correlated to obtain the following mass percent (1) equation:

$$\text{solubility}\ [100\,w_1] = -0.640\,93 + 3.087\,18\times10^{-3}(T/\text{K}),$$

which yielded a standard deviation of 7.67×10^{-3} in the temperature range from 275 to 303 K.

The curve obtained from the smoothing equation does not show a minimum over the temperature interval under examination as shown in Fig. 4. The conditions for the appearance of the solubility minimum are discussed in the Preface.

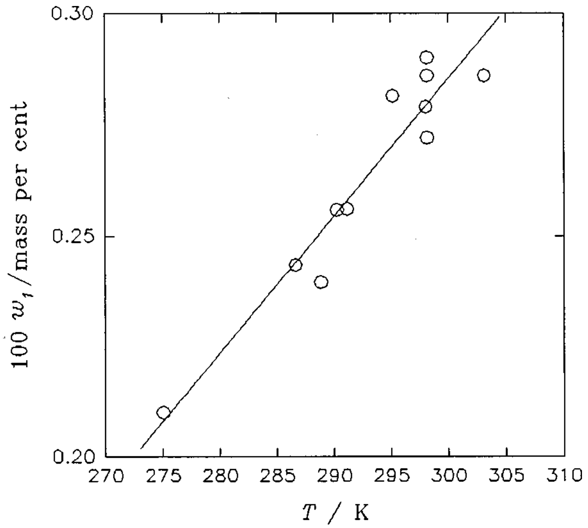

FIG. 4. Solubility of 1,3-dichloropropane (1) in water (2).

The tentative solubility values for this system in mass percent and mole fraction are given in Table 14, as smoothed values at 5 K intervals.

TABLE 14. Tentative solubility of 1,3-dichloropropane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^4\ x_1$
5	278.15	218×10^{-1}	3.48
10	283.15	2.33×10^{-1}	3.72
15	288.15	2.49×10^{-1}	3.98
20	293.15	2.64×10^{-1}	4.22
25	298.15	2.80×10^{-1}	4.48
30	303.15	2.95×10^{-1}	4.72

References:

[1] P. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
[2] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
[3] P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).
[4] B. G. Chitwood, Adv. Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).
[5] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
[6] G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Components:	**Original Measurements:**
(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9] (2) Water; H_2O; [7732-18-5]	P. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.273	0.272	4.35

Auxiliary Information

Method/Apparatus/Procedure:

A weighted amount of 1,3-dichloropropane was mixed with 1000 g water in a bottle and immersed in a water thermostat bath. The bottle was placed on a shaker and shaken until no more liquid droplets remained undissolved. The concentration of the 1,3-dichloropropane in water was determined by a Zeiss water interferometer. One or more samples were syphoned out for the solubility determination. The German translation also has been published.[1]

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K.

References:

[1] P. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Components:	**Original Measurements:**
(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	3.50×10^2	0.286	4.57

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,3-dichloropropane with a large volume of water and then measuring the volume of the undissolved portion of 1,3-dichloropropane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	2.87	0.286	4.57

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solution was prepared in a flask and placed in a waterbath thermostat. The samples were analyzed using a Zeiss combination liquid and gas interferometer described elsewhere.[1] A detailed description of the complete procedure is given in a MA thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Company, distilled fractionally before use. The b.p. range was 120.5–120.6 °C.
(2) Distilled.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[2] M. A. Gorman, MA thesis, Duke University, Durham, 1932.

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Adv. in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.29	4.64	2.57×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Adv. in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.29	4.64	2.57×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=275–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
1.9	17.71	0.2101	3.356
13.5	31.70	0.2434	3.889
15.7	36.21	0.2395	3.837
17.1	37.14	0.2558	4.087
22.0	44.97	0.2814	4.497
24.9	53.57	0.2789	4.458

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,3-dichloropropane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmater. The 1,3-dichloropropane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.0%.
Temperature: ±0.5 K.

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Variables:

T/K=291

Prepared By:

A. L. Horvath

Experimental Data

Water origin	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
De-ionized water	2.56±0.05	0.256	4.091
Artificial seawater	2.46±0.04	0.246	—
Mediterranean seawater	2.20±0.02	0.220	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,3-dichloropropane was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.

Estimated Errors:

Solubility: See above.
Temperature: ±1.0 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, G. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **11**, 178 (1983).

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Magnesium sulfate; $MgSO_4$; [7587-88-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

T/K=298
Concentration(2)/mol dm^{-3}=0.5

Prepared By:

A. L. Horvath

28. 1,3-Dichloropropane with Magnesium Sulfate and Water

Experimental Data

t/°C	c_2 /mol dm^{-3}	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.5	0.158	0.158	2.659

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10–20 cm^3 1,3-dichloropropane in 500 cm^3 of an aqueous $MgSO_4$ solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,3-dichloropropane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K.

Components:

(1) 1,3-Dichloropropane; $C_3H_6Cl_2$; [142-28-9]
(2) Potassium chloride; KCl; [3811-04-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

$T/\mathrm{K}=298$
Concentration(2)/mol $\mathrm{dm}^{-3}=0.5$

Prepared By:

A. L. Horvath

29. 1,3-Dichloropropane with Potassium Chloride and Water

Experimental Data

$t/°\mathrm{C}$	c_2 /mol dm^{-3}	100 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.5	0.230	0.230	3.781

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10–20 cm^3 1,3-dichloropropane in 500 cm^3 of an aqueous KCl solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,3-dichloropropane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.01 K.

Components:

(1) 1-Bromopropane; C_3H_7Br; [106-94-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

30. 1-Bromopropane with Water

Critical Evaluation

The solubility of 1-bromopropane (1) in water (2) has been studied by four work groups, whereas, the solubility of water (2) in 1-bromopropane (1) has not been investigated yet. The temperature dependence of the solubility between 273 and 303 K was reported in only one paper.[1]

Despite the small temperature difference among the measured solubilities, the agreement is reasonable. The available solubility data of Rex,[1] of Führer,[2] of Gross and Saylor,[3] and of van Arkel and Vles[4] were correlated to obtain the following mass percent (1) equation:

$$\text{solubility}\ [100\ w_1]=9.0608-0.059\,10\ (T/\mathrm{K})+9.8925\times10^{-5}\ (T/\mathrm{K})^2,$$

which yielded a standard deviation of 9.38×10^{-3} in the temperature range from 273 to 303 K. The curve obtained from the smoothing equation shows a distinct minimum at 298.7 K as shown in Fig. 5.

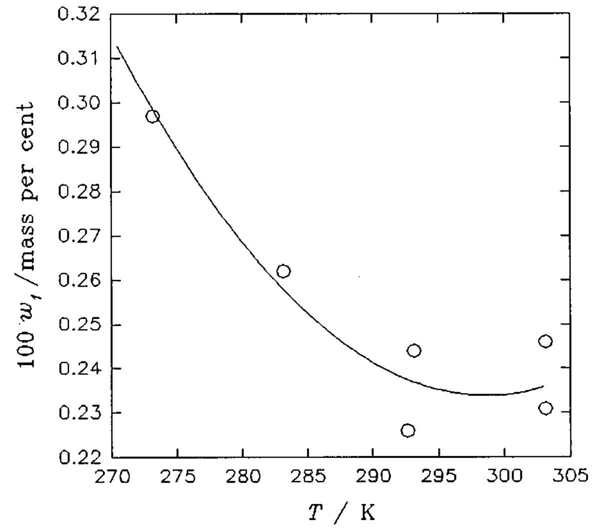

FIG. 5. Solubility of 1-bromopropane (1) in water (2).

The tentative solubility values for this system in mass percent and mole fraction are given in Table 15, as smoothed values at 5 K intervals.

TABLE 15. Tentative solubility of 1-bromopropane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^4\ x_1$
0	273.15	2.98×10^{-1}	4.38
5	278.15	2.76×10^{-1}	4.05
10	283.15	2.58×10^{-1}	3.79
15	288.15	2.45×10^{-1}	3.60
20	293.15	2.37×10^{-1}	3.48
25	298.15	2.34×10^{-1}	3.34
30	303.15	2.36×10^{-1}	3.46

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Fühner, Ber. **57**, 510 (1924).
[3] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[4] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Components:	**Original Measurements:**
(1) 1-Bromopropane; C_3H_7Br; [106-94-5] (2) Water; H_2O; [7732-18-5]	A. Rex, Z. Phys. Chem. **55**, 355 (1906).
Variables:	**Prepared By:**
T/K=273–303	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.298	0.297	4.36
10	0.263	0.262	3.85
20	0.245	0.244	3.58
30	0.247	0.246	3.61

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1-bromopropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b. p. was 70.8 °C.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Bromopropane; C_3H_7Br; [106-94-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. Fühner, Ber. **57**, 510 (1924).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1 M_1^{-1}$/mol g^{-1}
19.5	0.226	3.32	1.84×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

1-Bromopropane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-bromopropane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Bromopropane; C_3H_7Br; [106-94-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	2.31	0.231	3.39

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1-bromopropane in 500 g water was shaken for 12 h in a waterbath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph.D. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Company, purified by fractional distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
[2] J. H. Saylor, Ph.D. thesis, Duke University, Durham, 1930.

Components:
(1) 1-Bromopropane; C_3H_7Br; [106-94-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:
T/K=303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$10^3\ x_1$	$100\ n_1 g_2^{-1}$/mol g^{-1}	$100\ w_1$ (compiler)
30	0.339	1.88×10^{-3}	0.231

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 2-Bromopropane; C_3H_7Br; [75-26-3]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

31. 2-Bromopropane with Water

Critical Evaluation

The solubility of 2-bromopropane (1) in water (2) has been studied by three work groups; whereas, the solubility of water (2) in 2-bromopropane (1) has not been investigated yet. The temperature dependence of the solubility between 273 and 303 K was reported in only one paper.[1]

The datum of Fühner[2] is 10% lower than that of Rex[1] and of van Arkel and Vles.[3] Not enough workers have measured the solubility of 2-bromopropane in water over common temperature ranges to provide a basis for recommend solubility values. The solubility data of Rex[1] are believed to be more reliable than the other data because Rex made measurements at more than one temperature. All the results are considered to be tentative, but the data of Rex[1] are preferred by the evaluator. The tentative solubility values for this system in mass percent and mole fraction are given in Table 16 at 10 K intervals.

TABLE 16. Tentative solubility of 2-bromopropane (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^4\ x_1$
0	273.15	4.16×10^{-1}	6.11
10	283.15	3.64×10^{-1}	5.35
20	293.15	3.17×10^{-1}	4.66
30	303.15	3.17×10^{-1}	4.66

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Fühner, Ber. **57**, 510 (1924).
[3] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Components:
(1) 2-Bromopropane; C_3H_7Br; [75-26-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Rex, Z. Phys. Chem. **55**, 335 (1906)

Variables:
T/K=273–303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
0	0.418	0.416	6.11
10	0.365	0.364	5.35
20	0.318	0.317	4.66
30	0.318	0.317	4.66

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 2-bromopropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b. p. was 59 °C.
(2) Distilled.

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 2-Bromopropane; C_3H_7Br; [75-26-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. **57**, 510 (1924).

Variables:
T/K=291

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
18	0.286	4.20	2.32×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

2-Bromopropane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 2-bromopropane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-Bromopropane; C_3H_7Br; [75-26-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

$T/K = 303$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^3\ x_1$	$100\ n_1 g_2^{-1}$/mol g^{-1}	$100\ w_1$ (compiler)
30.0	0.468	2.6×10^{-3}	0.319

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,-Chloropropane; C_3H_7Cl; [540-54-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

32. 1-Chloropropane with Water

Critical Evaluation

The solubility of 1-chloropropane (1) in water (2) has been studied by five work groups, whereas the solubility of water (2) in 1-chloropropane (1) has not been investigated yet. The temperature dependence of the solubility of 1-chloropropane (1) in water (2) between 273 and 303 K was reported in only one paper.[1]

The data are in very poor agreement and further studies will be necessary before any values can be recommended. In the opinion of the evaluator, there is not enough evidence to justify rejection of any of the five available data sets. The three sets of data by Fühner,[2] by Wright and Schaffer,[3] and by Sato and Nakijima[4] are classed as doubtful; whereas, the data of Rex[1] and of van Arkel and Vles[5] are considered reliable and preferred for use. The solubility data of Rex[1] are believed to be more reliable than the other data because Rex made measurements at more than one temperature. Furthermore, the listed solubility data between 273 and 303 K show a solubility minimum at ambient temperature which is consistent with trends observed for halogenated hydrocarbon–water systems; see the Preface for more details.

All the reported data for the solubility of 1-chloropropane (1) in water (2) for the temperature range from 273 to 310 K in mass percent and mole fraction are summarized in Table 17.

TABLE 17. Reported solubility of 1-chloropropane (1) in water (2)

Temperature		Solubility		
°C	K	$100\ w_1$	$10^4\ x_1$	Reference
0	273.15	0.375	8.62	1
10	283.15	0.322	7.40	1
12.5	285.65	0.232	5.33	2
20	293.15	0.271	6.23	1
25	298.15	0.250	5.74	3
30	303.15	0.276	6.34	1
		0.277	6.36	5
37	310.15	0.244	5.62	4

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Fühner, Ber. **57**, 510 (1924).
[3] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
[4] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
[5] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bass **55**, 407 (1936).

Components:	**Original Measurements:**
(1) 1-Chloropropane; C_3H_7Cl; [540-54-5] (2) Water; H_2O; [7732-18-5]	A. Rex, Z. Phys. Chem. **55**, 355 (1906).
Variables:	**Prepared By:**
T/K=273–303	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
0	0.376	0.375	8.62
10	0.323	0.322	7.40
20	0.272	0.271	6.23
30	0.277	0.276	6.34

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1-chloropropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b.p. was 46.2 °C.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Chloropropane; C_3H_7Cl; [540-54-5] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables:	**Prepared By:**
T/K=286	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
12.5	0.232	5.33	2.95×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

1-Chloropropane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-chloropropane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Chloropropane; C_3H_7Cl; [540-54-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	4.00×10^2	0.250	5.74

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1-chloropropane with a large volume of water and then measuring the volume of the undissolved portion of 1-chloropropane.

Source and Purity of Materials:

(1) Prepared by the authors. Purified by treating with H_2SO_4, washed with $NaHCO_3$ solution and water. Dried with $CaCl_2$ before use.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Chloropropane; C_3H_7Cl; [540-54-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^3 x_1	100 $n_1 g_2^{-1}$/mol g^{-1}	100 w_1 (compiler)
30.0	0.636	3.53×10^{-3}	0.277

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Chloropropane; C_3H_7Cl; [540-54-5] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Water/air coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	1.1	0.244	5.62

[a] Gas–liquid partition parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1-chloropropane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.1 std. dev.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 2-Chloropropane; C_3H_7Cl; [75-29-6] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

33. 2-Chloropropane with Water

Critical Evaluation

The solubility of 2-chloropropane (1) in water (2) has been studied by three work groups, whereas the solubility of water (2) in 2-chloropropane (1) has not been investigated yet. The temperature dependence of the solubility between 273 and 303 K was reported in only one paper.[1]

Not enough workers measured the solubility of 2-chloropropane in water over common ranges of temperature to recommend solubility values. Although the data of Rex,[1] of Fühner,[2] and of van Arkel and Vles[3] are in good agreement, the solubility data of Rex[1] are believed to be more reliable than the other data because Rex made measurements at more than one temperature.

The tentative solubility of 2-chloropropane (1) in water (2) in the temperature range from 273 to 303 K in mass percent and mole fraction is listed in Table 18 at 10 K intervals. It is apparent that any solubility minimum should appear above 303 K. For further discussion on the solubility minimum in halogenated hydrocarbon–water systems, see the Preface for more details.

TABLE 18. Tentative solubility of 2-chloropropane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	4.38×10^{-1}	10.1
10	283.15	3.61×10^{-1}	8.30
20	293.15	3.04×10^{-1}	6.99
30	303.15	3.03×10^{-1}	6.97

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Fühner, Ber. **57**, 510 (1924).
[3] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Components:

(1) 2-Chloropropane; C_3H_7Cl; [75-29-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Rex, Z. Phys. Chem. **55**, 355 (1906).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.440	0.438	10.1
10	0.362	0.361	8.30
20	0.305	0.304	6.99
30	0.304	0.303	6.97

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 2-chloropropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b.p. was 34.8 °C.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-Chloropropane; C_3H_7Cl; [75-29-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. Fühner, Ber. **57**, 510 (1924).

Variables:

T/K=286

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
12.5	0.342	7.86	4.35×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

2-Chloropropane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 2-chloropropane added to a known quality of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-Chloropropane; C_3H_7Cl; [75-29-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $n_1 g_2^{-1}$/mol g^{-1}	$10^3 x_1$ (compiler)	100 w_1 (compiler)
30.0	3.9×10^{-3}	0.702	0.306

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Iodopropane; C_3H_7I; [107-08-4]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

34. 1-Iodopropane with Water

Critical Evaluation

The solubility of 1-iodopropane (1) in water (2) has been studied by four work groups, whereas the solubility of water (2) in 1-iodopropane (1) has not been investigated yet. The temperature dependence of the solubility between 273 and 303 K was reported in only one paper.[1]

Although all the data of Rex,[1] of Führer,[2] of Gross and Saylor,[3] and of Schwarz[4] are in good agreement, the solubility data of Rex are believed to be more reliable than the other data because Rex made measurements at more than one temperature.

All the available data for the solubility of 1-iodopropane (1) in water (2) were combined and correlated to obtain the following mass percent (1) equation:

$$\text{solubility } [100\, w_1] = 3.4659 - 0.023\,046\ (T/\text{K}) + 3.944\,24\times10^{-5}\ (T/\text{K})^2,$$

which yielded a standard deviation of 8.06×10^{-3} and represents the solubility behavior in the temperature range from 273 to 303 K. The temperature dependence of the solubility is illustrated in Fig. 6. The solubility curve derived from the above regression equation shows a solubility minimum at 292.15 K. More details on the appearance of a solubility minimum in halogenated hydrocarbon–water systems are discussed in the Preface.

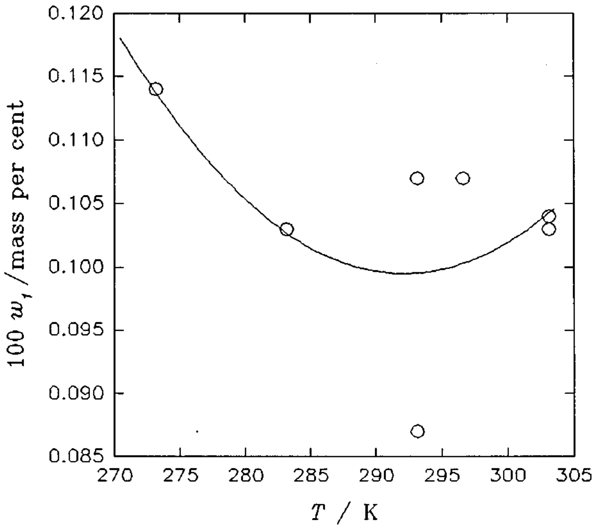

FIG. 6. Solubility of 1-iodopropane (1) in water (2).

The tentative solubility values for this system in mass percent and mole fraction are given in Table 19, as smoothed values at 5 K intervals.

TABLE 19. Tentative solubility of 1-iodopropane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	1.14×10^{-1}	1.21
5	278.15	1.07×10^{-1}	1.14
10	283.15	1.03×10^{-1}	1.09
15	288.15	1.00×10^{-1}	1.06
20	293.15	1.00×10^{-1}	1.06
25	298.15	1.01×10^{-1}	1.07
30	303.15	1.04×10^{-1}	1.10

References:

[1]A. Rex, Z. Phys. Chem. **55**, 355 (1906).

[2]H. Fühner, Ber. **57**, 510 (1924).

[3]P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

[4]F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:	**Original Measurements:**
(1) 1-Iodopropane; C_3H_7I; [107-08-4] (2) Water; H_2O; [7732-18-5]	A. Rex, Z. Phys. Chem. **55**, 355 (1906).
Variables: T/K=273–303	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
0	0.114	0.114	1.21
10	0.103	0.103	1.09
20	0.107	0.107	1.13
30	0.103	0.103	1.09

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1-iodopropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and their weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b.p. was 100.6 °C.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1-Iodopropane; C_3H_7I; [107-08-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. **57**, 510 (1924).

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	8.7×10^{-2}	9.23	5.12×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:
1-Iodopropone was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-iodopropane added to a known quality of water present.

Source and Purity of Materials:
(1) E. Merck, Darmstadt. Further purified before use.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1-Iodopropane; C_3H_7I; [107-08-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:
T/K=303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
30	1.04	0.104	1.10

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 1-iodopropane in 500 g water was shaken for 12 h in a waterbath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph.D. thesis.[2]

Source and Purity of Materials:
(1) Eastman Kodak Company, shaken with $Na_2S_2O_3$ solution and distilled water, and fractionated before use.
(2) Distilled.

Estimated Errors:
Solubility: ±3.0%.
Temperature: ±0.02 K.

References:
[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
[2] J. H. Saylor, Ph.D. thesis, Duke University, Durham, 1930.

Components:	**Original Measurements:**
(1) 1-Iodopropane; C_3H_7I; [107-08-4] (2) Water; H_2O; [7732-18-5]	F. P. Schwartz, Anal. Chem. **52**, 10 (1980).

Variables:	**Prepared By:**
T/K=297	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	$10\ w_1M_1^{-1}$/mol g^{-1} (compiler)
23.5	0.107	1.13	6.29×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous solubility was determined by elution chromatography. The solute columns (3 mm o.d., 2 mm i.d., 40 cm in length) were filled with Chromosorb P. The analysis involved the removal of the packing from the column segment into a test tube containing octane. The samples were injected into a gas chromatograph. The average deviations were calculated from several measurements from different samples.

Source and Purity of Materials:

(1) Commercial reagent of spectral grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±3% std. dev.
Temperature: ±1.5 K

Components:	**Original Measurements:**
(1) 1-Iodopropane; C_3H_7I; [75-30-9] (2) Water; H_2O; [7732-18-5]	A. Rex, Z. Phys. Chem. **55**, 355 (1906).

Variables:	**Prepared By:**
T/K=273–303	A. L. Horvath

35. 2-Iodopropane with Water

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.167	0.167	1.77
10	0.143	0.143	1.52
20	0.140	0.140	1.48
30	0.134	0.134	1.42

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 2-iodopropane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostat bath, their volumes and their weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use. The b.p. was 88.2 °C.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

36. 1,1,2,3,4,4-Hexachloro-1,3-butadiene with Water

Critical Evaluation

The 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) in water (2) and part 2 is water (2) in 1,1,2,3,4,4-hexachloro-1,3-butadiene (1).

Part 1. The solubility of 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) in water (2) has been studied by eight work groups in the temperature range from 288 to 313 K. The data are in very poor agreement and with the absence of other independent studies it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be proposed. All the available data for the solubility of 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) in water (2) in mass percent and mole fraction are summarized in Table 20.

TABLE 20. Reported solubility of 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^7 x_1	Reference
15	288.15	3.2×10^{-4}	2.21	1
20	293.15	5.0×10^{-4}	3.45	2
		3.8×10^{-4}	2.62	1
		2.0×10^{-4}	1.38	3
		2.0×10^{-4}	1.38	4
		6.075×10^{-4}	4.20	5
25	298.15	3.24×10^{-4}	2.20	6
		5.003×10^{-4}	3.46	7
26	299.15	4.12×10^{-4}	2.85	1
40	313.15	$59.\times10^{-4}$	40.8	8

Part 2. The solubility of water (2) in 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) has been reported in only four works from the same laboratory between 1970 and 1974. The agreement is sufficiently reliable to use in the smoothing equation. All the available data of Simonov *et al.*,[8] of Simonov *et al.*,[9] of Antropov *et al.*,[1] and of Simonov *et al.*[10] were used for fitting the smoothing equation of mole fraction solubility of water in 1,1,2,3,4,4-hexachloro-1,3-butadiene versus the reciprocal of absolute temperature.

$$\log_{10} x_2 = 11.2192 - 4379.80/(T/\mathrm{K}).$$

This equation, representing the combined data, yielded a standard deviation of 1.83×10^{-1} in the temperature range from 288 to 323 K. The tentative solubility values at 5 K intervals for water (2) in 1,1,2,3,4,4-hexachloro-1,3-butadiene (1) in weight percent and mole fraction are presented in Table 21.

TABLE 21. Tentative solubility of water (2) in 1,1,2,3,4,4-hexachloro-1,3-butadiene (1)

Temperature		Solubility	
°C	K	100 w_2	10^4 x_2
15	288.15	7.26×10^{-4}	1.05
20	293.15	1.31×10^{-3}	1.90
25	298.15	2.34×10^{-3}	3.38
30	303.15	4.07×10^{-3}	5.89
35	308.15	7.01×10^{-3}	10.1
40	313.15	1.19×10^{-2}	17.2
45	318.15	1.97×10^{-2}	28.4
50	323.15	3.23×10^{-2}	46.6

The linear relation between the solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature is illustrated in Fig. 7. The straight line behavior of such plots is characteristic of the solubility of water in halogenated hydrocarbons; this behavior is discussed in the Preface in greater detail.

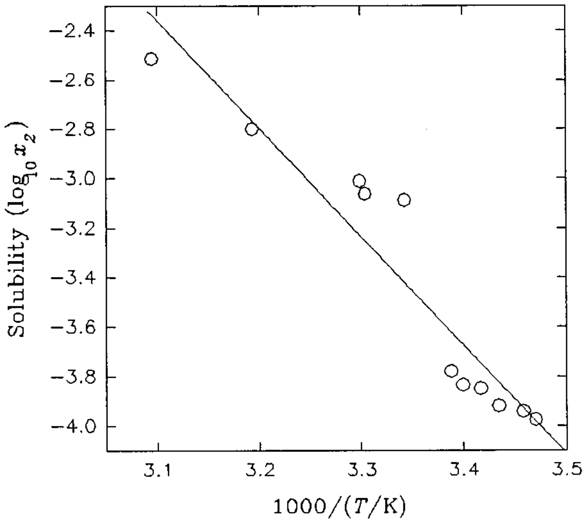

FIG. 7. Solubility of water (2) in 1,1,2,3,4,4-hexachloro-1,3-butadiene (1).

References:

[1] L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.

[2] E. T. McBee and R. E. Hatton, Ind. Eng. Chem. **41**, 809 (1949).

[3] G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).

[4] C. R. Pearson and G. McConnell, Proc. R. Soc. London, Ser. B **189**, 305 (1975).

[5] B. G. Oliver, Chemosphere **14**, 1087 (1985).

[6] S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

[7] H. P. Warner, J. M. Cohen, and J. C. Ireland, Determination of Henry's Law Constants of Selected Priority Pollutants, U. S. EPA Technical Report, PB87-212684, Cincinnati, OH (July, 1987).

[8] V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).

[9] V. D. Simonov V. E. Pogulyai, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **44**, 1755 (1970).

[10] V. D. Simonov *et al.*, Dokl. Neftekim. Sekt. Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 346 (1971).

Components:

(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. T. McBee and R. E. Hatton, Ind. Eng. Chem. **41**, 809 (1949).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^7\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	5.0×10^{-4}	3.45	1.9×10^{-6}

Auxiliary Information

Method/Apparatus/Procedure:

Details have been reported in a Ph.D. thesis.[1]

Source and Purity of Materials:

(1) Prepared by chlorination of polychlorobutane. The b.p. was 215 °C. At 20 °C, n_D=1.5542 and d_{20}=1.6820 g/cm^3.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.2 K (compiler).

References:

[1] R. E. Hatton, Ph. D. thesis, Purdue University, Lafayette, Ind., 1947.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]

Original Measurements:

V. D. Simonov, V. E. Pogulyai, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **44**, 1755 (1970).

Variables:

T/K=303–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
30	6.76×10^{-3}	9.78	3.75×10^{-4}
50	2.12×10^{-2}	30.60	1.18×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of water and 1,1,2,3,4,4-hexachloro-1,3-butadiene was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube as constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Synthesized by the authors, further purified by distillation.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]

Original Measurements:

V. D. Simonov *et al.*, Dokl. Neftekim. Sekt., Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 346 (1971).

Variables:

T/K = 288–303

Prepared By:

A. L. Horvath

Experimental Data

	$10^6 w_1$			$10^4 x_1$		
t/°C	Alekseev	Fischer	Spectroscopy	Alekseev	Fischer	Spectroscopy
15	7.12	7.42	7.42	1.030	1.074	1.074
16	7.80	7.83	8.20	1.129	1.133	1.187
19.5	9.74	9.82	9.89	1.410	1.421	1.431
21	10.2	—	10.1	1.476	—	1.462
29.5	59.9	59.6	—	8.663	8.620	—

Auxiliary Information

Method/Apparatus/Procedure:

The determination of the solubility of water in 1,1,2,3,4,4-hexachloro-1,3-butadiene was based on the infrared spectroscopic method. A UR-20 spectrophotometer was used with 2 cm cuvettes and the windows made of KBr. The spectra were recorded at 3600–810 cm^{-1}, and the absorbance at 3702 cm^{-1} was found by the baseline method. Standard mixtures of 1,1,2,3,4,4-hexachloro-1,3-butadiene and water were used for the calibration graphs. The results obtained were compared with the measurements made by the methods of cloud point[1] and a Karl Fischer titration.

Source and Purity of Materials:

(1) Distilled.
(2) Synthesized by the authors, distilled, washed with $HClSO_3$ and water, and distilled again. Dried with $CaCl_2$ and P_2O_5 before use.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K

References:

[1] V. F. Alekseev, Wied. Ann. **28**, 305 (1886).

Components:

(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.

Variables:

T/K = 288–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^7 x_1$ (compiler)	100 w_2	$10^4 x_2$ (compiler)
15	3.2×10^{-4}	2.21	—	—
18	—	—	0.834×10^{-3}	1.21
20	3.8×10^{-4}	2.62	—	—
22	—	—	1.25×10^{-3}	1.66
26	4.12×10^{-4}	2.85	5.65×10^{-3}	8.17

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of 1,1,2,3,4,4-hexachloro-1,3-butadiene and water was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Synthesized by the authors, purified by fractional distillation and dried with $CaCl_2$ and P_2O_5.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:	**Original Measurements:**
(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3] (2) Water; H_2O; [7732-18-5]	V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).
Variables:	**Prepared By:**
T/K=313	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^6\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
40	5.9×10^{-3}	4.08	1.10×10^{-2}	1.59

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination as described elsewhere[1] was used.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

References:

[1] V. D. Simonov, L. N. Popova, T. M. Shamsutdinov, V. I. Pogulyai, and F. A. Mamina, Symp. Doklay Neftekhimicheskoi Sektsii, Ufa. No. 6 (1971).

Components:	**Original Measurements:**
(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3] (2) Water; H_2O; [7732-18-5]	G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	100 w_1 (compiler)	$10^7\ x_1$ (compiler)
20	2.0	2.0×10^{-4}	1.38

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of the 1,1,2,3,4,4-hexachloro-1,3-butadiene in water was determined by gas–liquid chromatography (GLC) using an electron capture detector for analysis. Where possible, identification was confirmed by a linked mass spectrometer (MS) method.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.1 K (compiler).

Components:

(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. Pearson and G. McConnell, Proc. R. Soc. London Ser. B **189**, 305 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$10\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
2.0	2.0	2.0×10^{-4}	1.38

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with npentane and an aliquot of extract taken for gas–liquid chromatographic analysis. The gas chromatograph was fitted with a ^{63}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.1 K (compiler).

Components:

(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ c_1$/mol dm^3	$100\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
25	12.4	3.24×10^{-4}	2.20

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,2,3,4,4-hexachloro-1,3-butadiene was added to a stainless steel tube containing water and the tube was sealed. It was allowed to equilibrate during shaking for 1 week at 25 °C. After centrifugation, the sample was analyzed for radioactivity using a liquid scintillation counting. The solubility determination was repeated at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.3 K.

Components:	Original Measurements:
(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3] (2) Water; H_2O; [7732-18-5]	B. G. Oliver, Chemosphere **14**, 1087 (1985).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^7 x_1 (compiler)
20	43	6.08×10^{-4}	4.20

Auxiliary Information

Method/Apparatus/Procedure:

A gaseous purge system was used for the measurements. The apparatus consisted of a jacketed container which was thermostated in a water bath. The experiment was performed in the stripping apparatus by introducing 0.5 cm^3 of an acetone solution of 1,1,2,3,4,4-hexachloro-1,3-butadiene into 1 dm^3 water. The Henry's law constant was determined from the ratio of the concentration in the gas stream to concentration in the water.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.1 K.

Components:	Original Measurements:
(1) 1,1,2,3,4,4-Hexachloro-1,3-butadiene; C_4Cl_6; [87-68-3] (2) Water; H_2O; [7732-18-5]	H. P. Warner, J. M. Cohen, and J. C. Ireland, Determination of Henry's Law Constants of Selected Priority Pollutants, U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July, 1987).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^7 x_1 (compiler)
24.85	1.03×10^{-2}	5.0×10^{-4}	3.456

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described elsewhere,[1] was used. The general procedure was to add an excess quantity of 1,1,2,3,4,4-hexachloro-1,3-butadiene to distilled de-ionized water, place the sample in a thermostat bath, and mix overnight. A portion of this solution was returned to the stripping vessel. The 1,1,2,3,4,4-hexachloro-1,3-butadiene was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used without further purification. Stated purity >99%.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W.-Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) 2,3-Dichloro-1,3-butadiene; $C_4H_4Cl_2$; [1653-19-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Vojtko, M. Hrusovsky, and A. Kanala, Chemicke Zvesti. **21**, 443 (1967).

Variables:

T/K=293

Prepared By:

A. L. Horvath

37. 2,3-Dichloro-1,3-butadiene with Water

Experimental Data

t/°C	100 w_1	$10^5 x_1$ (compiler)	100 w_2	$10^2 x_2$ (compiler)
20	>0.02	>3.0	0.02	13.6

Auxiliary Information

Method/Apparatus/Procedure:

The titration method as described elsewhere[1] was used. Solubility data for the ternary system of water-methanol-2,3,-dichloro-1,3-butadiene were also reported.

Source and Purity of Materials:

(1) Synthesis was described elsewhere.[2] At 20 °C, $n_D = 1.4887$ and $d_4 = 1.1838$ g/cm^3.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1.0 K (compiler).

References:

[1] D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).
[2] W. H. Carothers and G. J. Berchett, J. Am. Chem. Soc. **55**, 2004 (1933).

Components:

(1) cis-,trans-1,4-Dichlorobutene; $C_4H_6Cl_2$; [31423-92-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Variables:

T/K=291

Prepared By:

A. L. Horvath

38. cis-,trans-1,4-Dichlorobutene with Water

Experimental Data

Water origin	ρ_1 /kg m^{-3}	100 w_1 (compiler)	$10^5 x_1$ (compiler)
Deionized water	0.598±0.006	5.98×10^{-2}	8.623
Artificial seawater	0.40±0.02	4.0×10^{-2}	—
Mediterranean seawater	0.35±0.02	3.5×10^{-2}	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of cis,-trans,-1,4-dichlorobutene was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.

Estimated Errors:

Solubility: See above.
Temperature: ±1.0 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **11**, 178 (1983).

Components:
(1) 4-Bromo-1-butene; C_4H_7Br; [5162-44-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data. **27**, 451 (1982).

Variables:
T/K=298

Prepared By:
A. L. Horvath

39. 4-Bromo-1-butene with Water

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	5.66×10^{-3}	7.63×10^{-2}	1.02

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 4-bromo-1-butene. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a high pressure liquid chromatographic method which has been described elsewhere.[1] The result is an average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

References:

[1] H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. **86**, 361 (1981).

Components:
(1) 4-Bromo-1-butene; C_4H_7Br; [5162-44-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	5.66	7.65×10^{-2}	1.02

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 4-bromo-1-butene. The saturated solution was then pumped through an extractor column and 4-bromo-1-butene was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,4-Dibromobutane; $C_4H_8Br_2$; [110-52-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Variables:

T/K=291

Prepared By:

A. L. Horvath

40. 1,4-Dibromobutane with Water

Experimental Data

Water origin	ρ_1 /kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
De-ionized water	0.35±0.03	3.5×10^{-2}	2.921
Artificial seawater	0.18±0.01	1.8×10^{-2}	—
Mediterranean seawater	0.162±0.006	1.62×10^{-2}	—

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,4-dibromobutane was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were prepared under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.

Estimated Errors:

Solubility: See above.
Temperature: ±1 K (compiler).

References:

[1] G. Bauduin, J. M. Bessiere, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis, **11**, 178 (1983).

Components:

(1) 1,1-Dichlorobutane; $C_4H_8Cl_2$; [541-33-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

41. 1,1-Dichlorobutane with Water

Experimental Data

t/°C	$V_2\ g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	2.0×10^3	5.01×10^{-2}	7.11

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,1-dichlorobutane with a large volume of water and then measuring the volume of the undissolved portion of 1,1-dichlorobutane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. T. Leighton and J. M. Calo, J. Chem. Eng. Data. **26**, 382 (1981).

Variables:
T/K=287–298

Prepared By:
A. L. Horvath

42. 1,4-Dichlorobutane with Water

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
13.5	15.27	0.1201	1.705
15.7	20.05	0.1044	1.482
17.1	21.35	0.1082	1.536
22.0	24.76	0.1283	1.822
24.9	26.61	0.1574	2.236

[a] Gas–liquid system analysis paramter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:
A 5 μL, 1,4-Dichlorobutane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,4-dichlorobutane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled.

Estimated Errors:
Solubility: ±6.1%.
Temperature: ±0.5 K.

Components:
(1) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. Bauduin, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis **13**, 124 (1985).

Variables:
T/K=291

Prepared By:
A. L. Horvath

Experimental Data

Water origin	ρ_1 /kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
De-ionized water	0.648±0.009	6.48×10^{-2}	9.196
Artificial seawater	0.67±0.08	6.7×10^{-2}	—
Mediterranean seawater	0.66±0.03	6.6×10^{-2}	—

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of 1,4-dichlorobutane was determined in three different aqueous solution types: de-ionized water and artificial and Mediterranean seawaters. The saturated solutions were presented under vigorous agitation from 4 to 5 h. After filtration, samples of the homogeneous aqueous phase were analyzed using gas chromatography. Further details on the analytical method are given elsewhere.[1]

Source and Purity of Materials:
(1) Source and purity not given.
(2) Source and purity not given.

Estimated Errors:
Solubility: See above.
Temperature: ±1 K (compiler).

References:
[1] G. Bauduin, J. M. Bessiere, D. Bondon, J. Gonzales-Moran, and Y. Pietrasanta, Analusis, **11**, 178 (1983).

Components:

(1) 2,3-Dichlorobutane; $C_4H_8Cl_2$; [7581-97-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. V. Likhosherstov, S. V. Alekseev, and T. V. Shalaeva, J. Chem. Ind. (Moscow) **12**, 705 (1935); CA 29:8174^5.

Variables:

T/K=173–313

Prepared By:

A. L. Horvath

43. 2,3-Dichlorobutane with Water

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
0	1.82×10^{-1}	2.585	—	—
18	—	—	0.17	1.187
20	5.62×10^{-2}	0.797	—	—
30	1.86×10^{-2}	0.264	—	—
40	2.23×10^{-2}	0.316	—	—

Auxiliary Information

Method/Apparatus/Procedure:

A More titration analysis or an adsorption indicator method was used for the determination of chlorides in the saturated aqueous solution of 2,3-dichlorobutane. An equal parts mixture (10 cm^3) of the sample and a NaOH solution was boiled for 4 h. After the sample was cooled, the chloride ions were titrated with $AgNO_3$ solution until all the silver chloride coagulated. The solubility was calculated from the volume of $AgNO_3$ solution used.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1-Bromo-2-methylpropane; C_4H_9Br; [78-77-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. Fühner, Ber. **57**, 510 (1924).

Variables:

T/K=291

Prepared By:

A. L. Horvath

44. 1-Bromo-2-methylpropane with Water

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
18	5.1×10^{-2}	6.71	3.72×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Bromo-2-methylpropane was added gradually from a pipette to 100 cm^{-3} water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-bromo-2-methylpropane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt. Further purified before use.
(2) Distiller (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

45. 1-Bromobutane with Water

Critical Evaluation

The solubility of 1-bromobutane (1) in water (2) has been studied by five work groups over the temperature range from 289 to 303 K. The data are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable.

The approximate single value of Booth and Everson[1] is considerably lower than all other measurements and is therefore rejected. Despite the narrow temperature difference between the solubility data of Fühner[2] and of Gross and Saylor[3] the agreement is good. However, the more recent measurements by Tewari *et al.*[4] and by Miller *et al.*[5] from the same laboratory resulted in much higher solubility values. There are no comparable data values at 18 and 30 °C.

Further studies will be necessary before even tentative values can be proposed. All the available data for the solubility of 1-bromobutane (1) in water (2) in mass percent and mole fraction are summarized in Table 22.

TABLE 22. Reported solubility of 1-bromobutane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^5\ x_1$	Reference
16	289.15	5.80×10^{-2}	7.63	2
25	298.15	$<2.56\times10^{-2}$	<3.37	1
25	298.15	8.68×10^{-2}	11.4	4
25	298.15	8.71×10^{-2}	11.46	5
30	303.15	6.08×10^{-2}	8.00	3

References:

[1] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

[2] H. Fühner, Ber. **57**, 510 (1924).

[3] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

[4] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[5] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables: T/K=289	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
16	5.8×10^{-2}	7.63	4.23×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Bromobutane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-bromobutane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt. Further purified before use.
(2) Distiller (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
Variables: T/K=303	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
30	0.608	6.08×10^{-2}	8.00

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1-bromobutane in 500 g water was shaken for 12 h in a waterbath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph.D. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Company. Purified by fractional distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: ±1.5%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
[2] J. H. Saylor, Ph.D. thesis, Duke University, Durham, 1930.

Components:	**Original Measurements:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	$100\ V_1/V_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25.0	<0.02	<0.0256	<3.37

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium was established through repeated shaking and centrifuging of a 1-bromobutane and water mixture in a stoppered Goetz tube and returned the tube to a constant temperature water bath. The difference between the total amount of 1-bromobutane which was added and the amount which remained in excess was the amount of solute dissolved in the known volume of water. The determination of the excess amount of solute added is described elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, C.P. grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: <100%.
Temperature: ±1 K (compiler).

References:

[1] R. S. Hanslick, Ph.D. thesis, Columbia University, 1935.

Components:	**Original Measurements:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data. **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	6.34×10^{-3}	8.68×10^{-2}	1.14

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromobutane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1-Bromobutane; C_4H_9Br; [109-65-9] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ, Sci. Technol. **19**, 522 (1985).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	6.34	8.71×10^{-2}	1.146

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromobutane. The saturated solution was then pumped through an extractor column and 1-bromobutane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Evaluator:**
(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

46. 1-Chlorobutane with Water

Critical Evaluation

The solubility of 1-chlorobutane (1) in water (2) has been studied by six work groups, see the compilation sheets immediately following this critical evaluation. Most of the solubility data are rather uncertain and are classified as doubtful. The solubility of water (2) in 1-chlorobutane (1) has not been investigated yet.

Generally, the data are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be prescribed. Although, it may be noticed that the solubility data of Leighton and Calo[1] are believed to be more reliable than other data by Fühner,[2] by Wright and Schaffer,[3] by Sato and Nakijima,[4] by Tewari *et al.*,[5] and by Miller *et al.*,[6] because they made measurements at more than one temperature. Nevertheless, all the reported data for the solubility of 1-chlorobutane (1) in water (2) in mass percent and mole fraction are summarized in Table 23.

TABLE 23. Reported solubility of 1-chlorobutane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
1.0	274.15	6.241×10^{-2}	1.2153	1
3.0	276.15	6.050×10^{-2}	1.1780	1
12.4	285.55	6.992×10^{-2}	1.3616	1
12.5	285.65	6.596×10^{-2}	1.2843	1
12.5	285.65	6.6×10^{-2}	1.28	2
17.9	291.05	7.115×10^{-2}	1.3855	1
19.1	292.25	7.014×10^{-2}	1.3659	1
22.7	295.85	7.331×10^{-2}	1.4276	1
23.0	296.15	7.458×10^{-2}	1.4524	1
25.0	298.15	5.90×10^{-2}	1.15	3
25.0	298.15	8.72×10^{-2}	1.70	5
25.0	298.15	8.75×10^{-2}	1.70	6
37.0	310.15	7.11×10^{-2}	1.385	4

References:

[1] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

[2] H. Fühner, Ber. **57**, 510 (1924).

[3] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

[4] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

[5] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[6] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables:	**Prepared By:**
T/K=286	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	10 $w_1M_1^{-1}$/mol g^{-1} (compiler)
12.5	6.6×10^{-2}	1.28	7.13×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Chlorobutane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-chlorobutane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt. Further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

$t/°C$	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.70×10^3	5.90×10^{-2}	1.15

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1-chlorobutane with a large volume of water and then measuring the volume of the undissolved portion of 1-chlorobutane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2)Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

$t/°C$	Water/air coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.86	7.11×10^{-2}	1.385

[a] Gas–liquid partition parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

1-Chlorobutane vapor was equilibrated in an airtight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.18 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=274–296

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
1.0	325.5	6.241×10^{-2}	1.2153
3.0	375.3	6.050×10^{-2}	1.1780
12.4	536.9	6.992×10^{-2}	1.3616
12.5	569.2	6.596×10^{-2}	1.2843
17.9	693.4	7.115×10^{-2}	1.3855
19.1	738.2	7.014×10^{-2}	1.3659
22.7	833.9	7.331×10^{-2}	1.4276
23.0	839.0	7.458×10^{-2}	1.4524

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1-chlorobutane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1-chlorobutane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±2.1%.
Temperature: ±0.5 K.

Components:

(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3]
(1) Water; H_2O; [7732-18-5]

Original Measurements:

Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25.0	9.43×10^{-3}	8.72×10^{-2}	1.70

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-chlorobutane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1-Chlorobutane; C_4H_9Cl; [109-69-3] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	9.43	8.75×10^{-2}	1.70

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-chlorobutane. The saturated solution was then pumped through an extractor column and 1-chlorobutane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Evaluator:**
(1) 2-Chlorobutane; C_4H_9Cl; [78-86-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

47. 2-Chlorobutane with Water

Critical Evaluation

The solubility of 2-chlorobutane (1) in water (2) has been studied by two work groups, whereas the solubility of water (2) in 2-chlorobutane (1) has not been investigated yet.

The solubility data of 2-chlorobutane (1) in water (2) over the temperature range from 275 to 298 K show a continuous increase in solubility with temperature. The data of Wright and Schaffer[1] and of Leighton and Calo[2] are relatively consistent and are classified as tentative. The solubility data of Leighton and Calo[2] are believed to be more reliable than the single value of Wright and Schaffer[1] because they made measurements at more than one temperature.

The two sets of data for the solubility of 2-chlorobutane (1) in water (2) were combined and correlated to obtain the following mass percent (1) equation:

$$\text{solubility } [100\ w_1] = 8.9653 - 0.061\,598\ (T/\text{K}) + 1.0678\times10^{-4}\ (T/\text{K})^2,$$

which yielded a standard deviation of 5.38×10^{-3} and represents the solubility behavior in the temperature range from 273 to 298 K. The temperature dependence of the solubility is illustrated in Fig. 8. The solubility curve derived from the above regression equation shows a solubility minimum at 288.4 K. More details on the appearance of a solubility minimum in halogenated hydrocarbon–water systems are discussed in the Preface.

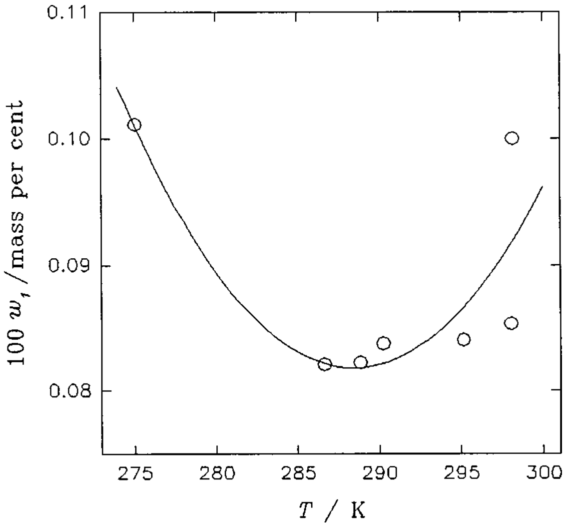

FIG. 8. Solubility of 2-chlorobutane (1) in water (2).

The tentative solubility values for this system in mass percent and mole fraction are given in Table 24, as smoothed values at 5 K intervals.

TABLE 24. Tentative solubility of 2-chlorobutane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	1.07×10^{-1}	2.08
5	278.15	9.3×10^{-2}	1.81
10	283.15	8.5×10^{-2}	1.65
15	288.15	8.2×10^{-2}	1.59
20	293.15	8.4×10^{-2}	1.64
25	298.15	$9.2\times10^{-}2$	1.79

References:

[1] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

[2] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Components:

(1) 2-Chlorobutane; C_4H_9Cl; [78-86-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.00×10^3	0.100	1.95

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 2-chlorobutane with a large volume of water and then measuring the volume of the undissolved portion of 2-chlorobutane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 2-Chlorobutane; C_4H_9Cl; [78-86-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:
T/K=275–298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
1.9	358.2	1.011×10^{-1}	1.969
13.5	773.6	8.211×10^{-2}	1.599
15.7	847.2	8.226×10^{-2}	1.602
17.1	891.0	8.375×10^{-2}	1.631
22.0	1109.3	8.405×10^{-2}	1.637
24.9	1243.3	8.534×10^{-2}	1.662

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:
A 5 μL 2-chlorobutane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 2-chlorobutane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled.

Estimated Errors:
Solubility: ±3.3%.
Temperature: ±0.5 K.

Components:
(1) 1-Chloro-2-methylpropane; C_4H_9Cl; [513-36-0]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

48. 1-Chloro-2-methylpropane with Water

Critical Evaluation

The 1-chloro-2-methylpropane (1) and water (2) binary system is treated in two parts; part 1 is 1-chloro-2-methylpropane (1) in water (2) and part 2 is water (2) in 1-chloro-2-methylpropane (1).

Part 1. The solubility of 1-chloro-2-methylpropane (1) in water (2) has been studied by two work groups with serious discrepancies. The value of Fühner[1] is an order of magnitude lower than that of Mackay *et al.*[2] The data are in very poor agreement and in the absence of other independent studies, it is not possible to determine which value is more reliable. Further studies will be necessary before even tentative values can be prescribed. All the available data for the solubility of 1-chloro-2-methylpropane (1) in water (2) in mass percent and mole fraction are summarized in Table 25.

TABLE 25. Reported solubility of 1-chloro-2-methylpropane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^4 x_1	Reference
12.5	285.65	9.2×10^{-2}	1.79	1
25	298.15	9.16×10^{-1}	17.96	2

Part 2. Only the value of Mackay *et al.*[2] is available for the solubility of water (2) in 1-chloro-2-methylpropane (1) at 298.15 K, and so no critical evaluation is possible. Further studies are required before any value can be recommended.

References:

[1] H. Fühner, Ber. **57**, 510 (1924).
[2] D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U.S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

Components:
(1) 1-Chloro-2-methylpropane; C_4H_9Cl; [513-36-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. **57**, 510 (1924).

Variables:
T/K=286

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	$10\ w_1M_1^{-1}$/mol g^{-1} (compiler)
1.25	9.2×10^{-2}	1.79	9.94×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Chloro-2-methylpropane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-chloro-2-methylpropane added to a known quantity of water present.

Source and Purity of Materials:
(1) E. Merck, Darmstadt. Further purified before use.
(2) Distilled (compiler).

Estimated Errors:
Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1-Chloro-2-methylpropane; C_4H_9Cl; [513-36-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay *et al.*, Volatilization of Organic Pollutants from Water, U.S. EPA Report 600/3-82-019, Athens, Georgia (1982); PB 82-230939.

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)	100 w_2 (compiler)	$10^3\ x_2$
25	99.0	0.916	1.796	7.81×10^{-2}	4.0

Auxiliary Information

Method/Apparatus/Procedure:

An aqueous solution with an excess amount of 1-chloro-2-methylpropane was stirred for 1 day before being introduced into a 1 L glass vessel. Nitrogen entered at the bottom of the vessel through a sintered glass disk. The exit glass flow rate was measured by a soap bubble flow meter. The concentration of 1-chloro-2-methylpropane in water was determined by gas chromatography. The GC was equipped with both a dual flame ionization detector and an electron capture detector.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Double distilled.

Estimated Errors:
Solubility: Not specified.
Temperature: ±1.0 K.

Components:

(1) 2-Chloro-2-methylpropane; C_4H_9Cl; [507-20-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. A. Clarke, T. R. Williams, and R. W. Taft, J. Am. Chem. Soc. **84**, 2292 (1962).

Variables:

T/K=274–288

Prepared By:

A. L. Horvath

49. 2-Chloro-2-methylpropane with Water

Experimental Data

t/°C	Partition coefficient,[a] K_L /mol m^{-3} atm^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
0.99	81.8±3.5	0.752	1.47
5.00	66.2±2.5	0.609	1.19
14.85	31.1±1.7	0.287	0.56

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

Both solute and solvent were degassed before their introduction into the reaction flask where the solute was vaporized. The system was then completely immersed in a thermostat bath. The flask was shaken to attain equilibrium. Manometer readings were taken at the calibrated temperatures. The distribution constants were calculated from the monitored readings and the apparatus calibration parameters.

Source and Purity of Materials:

(1) Prepared by the authors. The b.p. was 49.0 °C at 732 mm Hg.
(2) Triply distilled.

Estimated Errors:

Solubility: See above.
Temperature: ±0.02 K.

Components:

(1) 2-Chloro-2-methylpropane; C_4H_9Cl; [507-20-0]
(2) Water-d$_2$; D_2O; [7789-20-0]

Original Measurements:

G. A. Clarke, T. R. Williams, and R. W. Taft, J. Am. Chem. Soc. **84**, 2292 (1962).

Variables:

T/K=288

Prepared By:

A. L. Horvath

50. 2-Chloro-2-methylpropane with Water-d_2

Experimental Data

t/°C	Partition coefficient,[a] K_L /mol m^{-3} atm^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
14.85	31.8±1.1	0.265	5.168

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

Both solute and solvent were degassed before their introduction into the reaction flask where the solute was vaporized. The system was then completely immersed in a thermostat bath. The flask was shaken to attain equilibrium. Manometer readings were taken at the calibrated temperatures. The distribution constants were calculated from the monitored readings and the apparatus calibration parameters.

Source and Purity of Materials:

(1) Prepared by the authors. The b.p. was 49.0 °C at 732 mm Hg.
(2) Liquid Carbonic, 99.5% pure.

Estimated Errors:

Solubility: See above.
Temperature: ±0.02 K.

Components:	**Original Measurements:**
(1) 1-Iodobutane; C_4H_9Cl; [542-69-8] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables:	**Prepared By:**
T/K=291	A. L. Horvath

51. 1-Iodobutane with Water

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	10 $w_1M_1^{-1}$/mol g^{-1} (compiler)
17.5	2.1×10^{-2}	2.06	1.14×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Iodobutane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-iodobutane added to a known quality of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt. Further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1,1,2,3,4,5,5,5-Octachloro-1,3-pentadiene; C_5Cl_8; [1888-73-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

52. 1,1,2,3,4,5,5,5-Octachloro-1,3-pentadiene with Water

Critical Evaluation

The 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) in water (2) and part 2 is water (2) in 1,1,2,3,4,5,5,5-octa-chloro-1,3-pentadiene (1).

Part 1. The solubility of 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) in water (2) has been studied by two work groups from the same laboratory. The data at the lower temperatures appear to be inconsistent with the single high temperature value. Whether or not the two sets of data at different temperatures are consistent still must be established. The temperature dependence of the solubility observed by Simonov *et al.*[1] in the 313 K range is considerably higher than that of Antropov *et al.*[2] Nevertheless, there are insufficient independent data at present to justify exclusion of any values and thus all solubility results in mass percent and mole fraction are included in Table 26. In view of the lack of better consistency between the two sets of measurements, the listed values should be regarded as very tentative. The temperature dependence of the solubility of 1,1,2,3,4,5,5,5-octachloro-1,3-pentadine (1) in water (2) requires a thorough investigation over the whole temperature range in order to establish more reliable values.

TABLE 26. Tentative solubility of 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^9\ x_1$	Reference
15	288.15	1.44×10^{-5}	7.55	2
20	293.15	2.02×10^{-5}	10.59	2
26	299.15	3.40×10^{-5}	17.82	2
40	313.15	6.00×10^{-4}	314.0	1

Part 2. The solubility of water (2) in 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) has been reported by the same investigators who studied the solubility of 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1) in water (2).

The data consistency was studied by plotting $\log_{10} x_2$ versus the reciprocal of absolute temperature; see Fig. 9. The plot shows that the temperature dependence of the solubility observed by Antropov *et al.*[2] and by Simonov *et al.*[1] is sufficiently consistent over the temperature range from 291 to 313 K. Nevertheless, there are insufficient independent data at present to justify the recommendation of any values. All the reported values were correlated with the smoothing equation between 291 and 313 K:

$$\log_{10} x_2 = 5.2285 - 3113.03/(T/\mathrm{K}).$$

This equation yielded a standard deviation of 2.18×10^{-2} in the temperature range from 291 to 313 K.

A linear relation between the solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature is apparent in Fig. 9. The straight line behavior of such plots is characteristic of the solubility of water in halogenated hydrocarbons; this behavior is discussed in the Preface in greater detail.

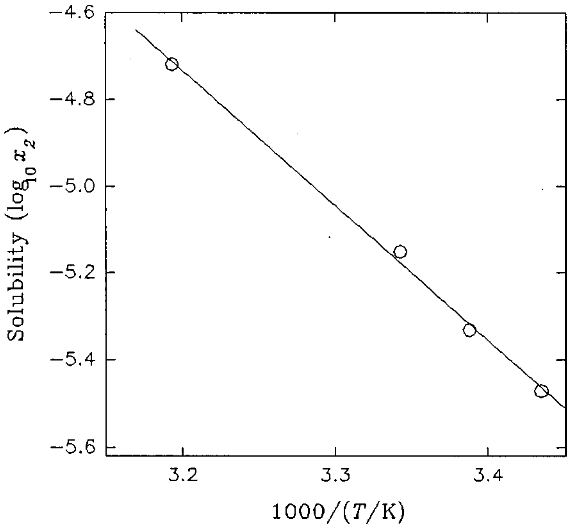

FIG. 9. Solubility of water (2) in 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1).

The tentative solubility values at 5 K intervals for water (2) in 1,1,2,3,4,5,5,5-octahloro-1,3-pentadiene (1) in mass percent and mole fraction are presented in Table 27.

TABLE 27. Tentative solubility of water (2) in 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene (1)

Temperature		Solubility	
°C	K	100 w_2	$10^5 x_2$
20	293.15	2.132×10^{-5}	0.4067
25	298.15	3.212×10^{-5}	0.6128
30	303.15	4.776×10^{-5}	0.9111
35	308.15	7.009×10^{-5}	1.337
40	313.15	10.185×10^{-5}	1.943

References:

[1]V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).

[2]L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.

Components:	**Original Measurements:**
(1) 1,1,2,3,4,5,5,5-Octachloro-1,3-pentadiene; C_5Cl_8; [1888-73-9] (2) Water; H_2O; [7732-18-5]	L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972); VINITI No. 3739-71.
Variables:	**Prepared By:**
T/K=288–299	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^9 x_1$ (compiler)	100 w_2	$10^6 x_1$ (compiler)
15	1.44×10^{-5}	7.55	—	—
18	—	—	1.77×10^{-5}	3.38
20	2.02×10^{-5}	10.59	—	—
22	—	—	2.45×10^{-5}	4.67
26	3.40×10^{-5}	17.82	3.69×10^{-5}	7.07

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of water and 1,1,2,3,4,5,5,5-octachloro-1,3-pentadiene was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Synthesized by the investigators, purified by fractional distillation and dried with $CaCl_2$ and P_2O_5.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1]W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) 1,1,2,3,4,5,5,5-Octachloro-1,3-pentadiene; C_5Cl_9; [1888-73-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).

Variables:

T/K=313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^7\ x_1$ (compiler)	100 w_1	$10^5\ x_2$ (compiler)
40	6.0×10^{-4}	3.14	1.0×10^{-4}	1.91

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alexejew was used. Further details are found elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] V. D. Simonov, L. N. Popova, T. M. Shamsutdinov, V. I. Pogulyai, and F. A. Mamina, Symp. Doklay Neftekhimicheskoi Sektsii, Ufa. No. 6 (1971).

Components:

(1) Dodecafluoropentane; C_5F_{12}; [678-26-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

53. Dodecafluoropentane with Water

Critical Evaluation

The solubility of dodecafluoropentane (1) in water (2) has been studied by two work groups from the same laboratory; whereas, the solubility of water (2) in dodecafluoropentane (1) has not been investigated yet.

The two sources of data, that of Kabal'nov *et al.*[1] and that of Kabalnov *et al.*,[2] are at the same temperature so a direct comparison of the measured values is possible. The two available data sets, measured at 298.15 K, are within 6% of each other.

Because it is not possible to say which of the two sets of measurements is more accurate, it is suggested that an average of the two is probably the most satisfactory. The average value provided in mass percent and mole fraction in Table 28 is considered tentative.

TABLE 28. Tentative solubility of dodecafluoropentane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^8\ x_1$
25	298.15	1.19×10^{-4}	7.43

It is apparent that the available measurements for this system can only be called sketchy, and that many more measurements are required to produce definitive solubility data.

References:

[1] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).
[2] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Flourine Chem. **50**, 271 (1990).

Components:	Original Measurements:
(1) Dodecafluoropentane; C_5F_{12}; [678-26-2] (2) Water; H_2O; [7732-18-5]	A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidn. Zh. **52**, 1060 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	V_1 /V_2	100 w_1 (compiler)	10^8 x_1 (compiler)
25	7.52×10^{-7}	1.227×10^{-4}	7.67

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of dodecafluoropentane in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of the coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent, 98% pure, passed through a column with Al_2O_3 before use.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:	Original Measurements:
(1) Dodecafluoropentane; C_5F_{12}; [678-26-2] (2) Water; H_2O; [7732-18-5]	A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine. Chem. **50**, 271 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^8 x_1 (compiler)
25	4.0×10^{-6}	1.15×10^{-4}	7.20

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of the particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Commercial grade, 98% pure. Source not given.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:

(1) 2,3-Dichloro-2-methylbutane; $C_5H_{10}Cl_2$; [507-45-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

54. 2,3-Dichloro-2-methylbutane with Water

Experimental Data

t/°C	$V_2g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	3.50×10^3	2.86×10^{-2}	3.65

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 2,3-dichloro-2-methylbutane with a large volume of water and then measuring the volume of the undissolved portion of 2,3-dichloro-2-methylbutane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-Dichloropentane; $C_5H_{10}Cl_2$; [1674-33-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

55. 1,2-Dichloropentane with Water

Experimental Data

t/°C	$V_2g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	3.50×10^3	2.86×10^{-2}	3.65

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,2-dichloropentane with a large volume of water and then measuring the volume of the undissolved portion of 1,2-dichloropentane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,5-Dichloropentane; $C_5H_{10}Cl_2$; [628-76-2] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=274–296	A. L. Horvath

56. 1,5-Dichloropentane with Water

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^5 x_1 (compiler)
1.0	16.36	1.170×10^{-2}	1.4949
3.0	23.10	9.763×10^{-3}	1.2472
12.4	21.41	2.214×10^{-2}	2.8282
12.5	28.87	1.642×10^{-2}	2.0974
17.9	26.96	2.635×10^{-2}	3.3668
19.1	36.69	2.080×10^{-2}	2.6579
22.7	79.33	1.232×10^{-2}	1.5732

Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,5-dichloropentane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,5-dichloropentane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±12.9%.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 2,3-Dichloropentane; $C_5H_{10}Cl_2$; [600-11-3] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

57. 2,3-Dichloropentane with Water

Experimental Data

t/°C	$V_2g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	3.50×10^3	2.86×10^{-2}	3.65

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 2,3-dichloropentane with a large volume of water and then measuring the volume of the undissolved portion of 2,3-dichloropentane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1-Bromo-3-methylbutane; $C_5H_{11}Br$; [107-82-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. **57**, 510 (1924).

Variables:
$T/K=290$

Prepared By:
A. L. Horvath

58. 1-Bromo-3-methylbutane with Water

Experimental Data

$t/°C$	$100\ w_1$	$10^5\ x_1$ (compiler)	$100\ w_1M_1^{-1}$/mol g^{-1} (compiler)
16.5	2.0×10^{-2}	2.39	1.32×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

1-Bromo-3-methylbutane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the 1-bromo-3-methylbutane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1-Bromopentane; $C_5H_{11}Br$; [110-53-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

59. 1-Bromopentane with Water

Critical Evaluation

The solubility of 1-bromopentane (1) in water (2) has been studied by two work groups in the same laboratory, where the solubility of water (2) in 1-bromopentane (1) has not been investigated yet.

The two experimental determinations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite satisfactory.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-bromopentane (1) in water (2) in mass percent, mole fraction, and mole per 100 g given in Table 29 is tentative and based primarily on the reported values of Tewari *et al.*[1] and of Miller *et al.*[2] at 298.15 K.

TABLE 29. Tentative solubility of 1-bromopentane (1) in water (2)

Temperature		Solubility		
°C	K	$100\ w_1$	$10^5\ x_1$	$100\ w_1M_1^{-1}$/mol g−1
25	298.15	1.27×10^{-2}	1.51	8.38×10^{-4}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromopentane; $C_5H_{11}Br$; [110-53-2] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25.0	8.38×10^{-4}	1.27×10^{-2}	1.51

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromopentane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector. The result is an average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1-Bromopentane; $C_5H_{11}Br$; [110-53-2] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	0.838	1.27×10^{-2}	1.51

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromopentane. The saturated solution was then pumped through an extractor column and 1-bromopentane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

60. 1-Chloropentane with Water

Critical Evaluation

The 1-chloropentane (1) and water (2) binary system is treated in two parts; part 1 is 1-chloropentane (1) in water (2) and part 2 is water (2) in 1-chloropentane (1).

Part 1. The solubility of 1-chloropentane (1) in water (2) has been studied by four work groups, whereas the solubility of water (2) in 1-chloropentane (1) has been reported in only one paper. The reported value of Booth and Everson[1] is significantly higher than other measurements and is therefore rejected. The remaining data of Wright and Schaffer,[2] of Sato and Nakijima,[3] and of Leighton and Calo[4] were combined and correlated to obtain the following mass percent (1) equation:

$$\text{solubility}\ [100\ w_1] = 0.557\,26 - 3.7269\times10^{-3}\ (T/\text{K}) + 6.457\times10^{-6}\ (T/\text{K})^2.$$

This equation, which represents the combined data values, yielded a standard deviation of 5.27×10^{-4} and represents the solubility behavior in the temperature range from 276 to 310 K. The temperature dependence of the solubility is illustrated in Fig. 10. The solubility curve derived from the above regression equation shows a distinct solubility minimum at 288.6 K as seen in Fig. 10. More details on the appearance of a solubility minimum in halogenated hydrocarbon–water systems are discussed in the Preface.

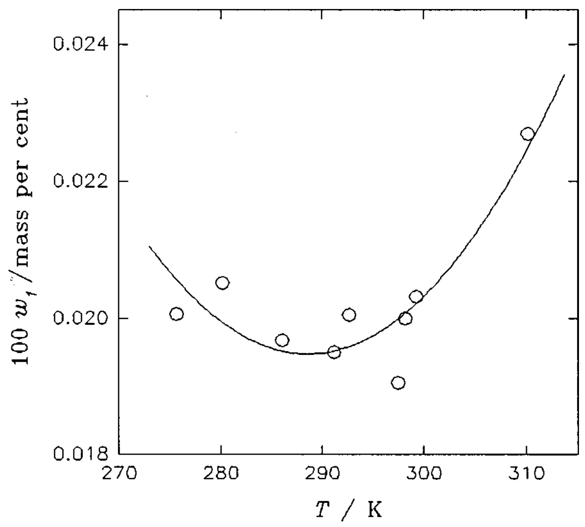

FIG. 10. Solubility of 1-chloropentane (1) in water (2).

The tentative solubility values at 5 K intervals for 1-chloropentane (1) in water (2) in mass percent and mole fraction are presented in Table 30.

TABLE 30. Tentative solubility of 1-chloropentane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^5x_1
5	278.15	2.02×10^{-2}	3.41
10	283.15	1.97×10^{-2}	3.33
15	288.15	1.95×10^{-2}	3.30
20	293.15	1.96×10^{-2}	3.31
25	298.15	2.01×10^{-2}	3.40
30	303.15	2.09×10^{-2}	3.53
35	308.15	2.20×10^{-2}	3.72

Part 2. The solubility of water (2) in 1-chloropentane (1) has been reported only by Hutchison and Lyon;[5] therefore, no critical evaluation can be made. The interested user is referred to the appropriate compilation sheet for the solubility value at 298.15 K. The measurement is classified as tentative since no other data are available.

References:

[1] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[2] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
[3] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
[4] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
[5] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Components:

(1) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2\ g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	5.00×10^3	2.00×10^{-2}	3.38

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1-chloropentane with a large volume of water and then measuring the volume of the undissolved portion of 1-chloropentane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	2.53×10^{-3}	4.56×10^{-2}	2.69

Auxiliary Information

Method/Apparatus/Procedure:

At 1 to 15 volume ratio mixture of water and 1-chloropentane was introduced into an equilibration flask and then lowered into the waterbath thermostat. The assembly was shaken mechanically for about 90 min at a constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.05 K.

References:

[1] M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey, eds., *Production of Heavy Water* (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

Experimental Data

$/t$°C	100 V_1/V_2	100 w_1 (compiler)	$10^4 x_1$ (compiler)
25.0	9.0×10^{-2}	7.9×10^{-2}	1.3

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium was established through repeated shaking and centrifuging of a 1-chloropentane and water mixture in a stoppered Goetz tube and returned the tube to a constant temperature water bath. The difference between the total amount of 1-chloropentane which was added and the amount which remained in excess was the amount of solute dissolved in the known volume of water. The determination of the excess amount of solute added is described elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, C.P. grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

References:

[1] R. S. Hanslick, Ph.D. thesis, Columbia University, 1935.

Components:

(1) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

$T/K=310$

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Water/air coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	$10^5 x_1$ (compiler)
37	0.70	2.27×10^{-2}	3.838

[a] Gas–liquid partition parameter; from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

1-Chloropentane vapor was equilibrated in an airtight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.19 std. dev.
Temperature: ±0.5 K (compiler)

Components:	**Original Measurements:**
(1) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=276–299	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^5 x_1 (compiler)
2.5	362.4	2.006×10^{-2}	3.3913
7.0	464.2	2.052×10^{-2}	3.4681
12.9	683.0	1.968×10^{-2}	3.3259
18.0	906.6	1.950×10^{-2}	3.2955
19.5	955.2	2.005×10^{-2}	3.3884
24.3	1302.6	1.906×10^{-2}	3.2219
26.1	1318.2	2.032×10^{-2}	3.4348

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1-chloropentane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1-chloropentane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±3.3%.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Water-d$_2$; D_2O; [7789-20-0] (2) 1-Chloropentane; $C_5H_{11}Cl$; [543-59-9]	C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

61. 1-Chloropentane with Water-d_2

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	2.22×10^{-3}	4.45×10^{-2}	2.36

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and 1-chloropentane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.05 K.

References:

[1] M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey, eds., *Production of Heavy Water* (McGraw-Hill, New York, 1955), p. 129.

Components:	Original Measurements:
(1) 2-Chloro-2-methylbutane; $C_5H_{11}Cl$; [594-36-5] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

62. 2-Chloro-2-methylbutane with Water

Experimental Data

t/°C	$V_2\ g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	3.00×10^2	0.333	5.64

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 2-chloro-2-methylbutane with a large volume of water and then measuring the volume of the undissolved portion of 2-chloro-2-methylbutane.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components	Original Measurements:
(1); $C_5H_{11}Cl$; [625-29-6] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

63. 2-Chloropentane with Water

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	4.00×10^3	2.51×10^{-2}	4.24

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 2-chloropentane with a large volume of water and then measuring the volume of the undissolved portion of 2-chloropentane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 3-Chloropentane; $C_5H_{11}Cl$; [616-20-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:
$T/\mathrm{K}=298$

Prepared By:
A. L. Horvath

64. 3-Chloropentane with Water

Experimental Data

$t/°\mathrm{C}$	$V_2 g_1^{-1}/\mathrm{cm^3\ g^{-1}}$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	4.00×10^3	2.51×10^{-2}	4.24

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 3-chloropentane with a large volume of water and then measuring the volume of the undissolved portion of 3-chloropentane.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(trifluoromethyl)-pentane; C_6F_{14}; [355-04-4]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

65. 1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(trifluoromethyl)-pentane with Water

Critical Evaluation

The solubility of 1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)-pentane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)-pentane (1) has not been investigated yet.

The two experimental determinations by Kabal'nov *et al.*[1] and by Kabalnov *et al.*[2] are in reasonable agreement, although further studies are required before any values can be recommended. Because it is not possible to say which of the two values is more accurate, it is suggested that the average of the two is probably the most reliable. The average value presented in Table 31 in mass percent and mole fraction is classified as tentative.

TABLE 31. Tentative solubility of 1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)-pentane (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^9\ x_1$
25	298.15	1.71×10^{-5}	9.09

References:

[1] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

[2] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

Components:

(1) 1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(trifluoromethyl)-pentane; C_6F_{14}; [355-04-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidn. Zh. **52**, 1060 (1990).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^9 x_1 (compiler)
25	1.02×10^{-5}	1.72×10^{-5}	9.17

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,1,1,2,2,3,3,4,5,5,5-undeca-fluoro-4-(trifluoromethyl)-pentane in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of the coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent, 97% pure, passed through a column with Al_2O_3 before use.
(2) Double distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:

(1) 1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(trifluoromethyl)-pentane; C_6F_{14}; [355-04-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^9 x_1 (compiler)
25	5.0×10^{-7}	1.69×10^{-5}	9.01

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial grade, 97% pure.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1.0 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:	**Evaluator:**
(1) Tetradecafluorohexane; C_6F_{14}; [355-42-0] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

66. Tetradecafluorohexane with Water

Critical Evaluation

The tetradecafluorohexane (1) and water (2) binary system is treated in two parts; part 1 is tetradecafluorohexane (1) in water (2) and part 2 is water (2) in tetradecafluorohexane (1).

Part 1. The solubility of tetradecafluorohexane (1) in water (2) has been studied by four work groups in the same laboratory between 1987 and 1990. It is probably safe to assume the data of Markina *et al.*[1] and of Markina *et al.*[2] have been superseded by those of Kabalnov *et al.*[3] and of Kabal'nov *et al.*,[4] since all four sets of measurements were made in the same laboratory.

The two sets of data, the earlier works of Markina *et al.*[1,2] and the later measurements by Kabalnov *et al.*[3,4] differ substantially by a factor of 3000. However, comparison of the trends in the solubility of perfluorohydrocarbons in water definitely indicate the lower value of Kabalnov *et al.*[3,4] should be preferred. Furthermore, because it is not possible to say which of the two[3,4] is more accurate, it is suggested that the average of the two, which is recorded in Table 32 in mass percent and mole fraction, is probably the most reliable.

TABLE 32. Tentative solubility of tetradecafluorohexane (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^9\ x_1$
25	298.15	0.978×10^{-5}	5.20

Part 2. Only the data of Shields[5] are available for the solubility of water (2) in tetradecafluorohexane (1); therefore, no critical evaluation is possible. These data are classified as tentative since no other data are available.

References:

[1] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

[2] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. im. D. I. Mendeleeva **33**, 344 (1988).

[3] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

[4] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

[5] R. R. Shields, J. Electrochem. Soc. **123**, 254C (1976).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Tetradecafluorohexane; C_6F_{14}; [355-42-0]	R. R. Shields, J. Electrochem. Soc. **123**, 254C (1976).
Variables:	**Prepared By:**
$T/\mathrm{K}=275-325$	A. L. Horvath

Experimental Data

The temperature dependence of the solubility of water in tetradecafluorohexane versus absolute temperature is expressed by the equation:

$$C_T=0.053\,253[\exp(417\,909.2/(T/\mathrm{K})^2-5999.96/(T/\mathrm{K})+7.283\,68)]$$

where C_T=solubility of water, g_1/g_2, and T=absolute temperature. For example, $C_T=0.001\,55[100\ g_1/g_2]$ at 298.15 K (compiler).

The above expression is not in the published abstract. The compiler obtained it direct from the author. In the communication, the author expressed the solubility in $\mu g_1/g_2$, which should read g_1/g_2, as given above.

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
Details are not available.	(1) Distilled (compiler). (2) Source and purity not given.
	Estimated Errors: Solubility: Not specified. Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Tetradecafluorohexane; C_6F_{14}; [355-42-0] (2) Water; H_2O; [7732-18-5]	Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidn, Zh. **49**, 1084 (1987).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^5\ x_1$	c_1 /mol dm^{-3}	100 w_1
19.85	1.6	9.0×10^{-4}	3.0×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of tetradecafluorohexane in water was determined through the use of precision tensiometric measurements for aqueous solutions of perfluorononane acid on its interface with perfluorodecalin at 298 K. The measurements served as a basis for evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from the water phase into a perfluoroorganic liquid phase.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Tetradecafluorohexane; C_6F_{14}; [355-42-0] (2) Water; H_2O; [7732-18-5]	Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. im. D. I. Mendeleeva **33**, 344 (1988).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^5\ x_1$	c_1 /mol dm^{-3}	100 w_1
20	1.6	9.0×10^{-4}	3.0×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The colloid chemical method was used for observing the shift in the critical micelle concentration formation for a surfactant in aqueous solutions under the influence of halogenated hydrocarbons. The solubility was calculated from the increment of standard chemical potential for the transfer of a fluoromethylene group from water into the fluorocarbon phase on the basis of experimental determination of the surface activity of a perfluoroorganic surface active nonelectrolyte.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) Tetradecafluorohexane; C_6F_{14}; [355-42-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^9 x_1 (compiler)
25	2.7×10^{-7}	9.13×10^{-6}	4.86

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial grade, 99% pure.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1.0 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:

(1) Tetradecafluorohexane; C_6F_{14}; [355-42-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidn. Zh. **52**, 1060 (1990).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^9 x_1 (compiler)
25	6.18×10^{-6}	1.042×10^{-5}	5.55

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of tetradecafluorohexane in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of the coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent. 99% pure, passed through a column with Al_2O_3 before use.
(2) Double distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:	**Evaluator:**
(1) 1-Bromohexane; $C_6H_{13}Br$; [111-25-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

67. 1-Bromohexane with Water

Critical Evaluation

The solubility of 1-bromohexane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1-bromohexane (1) has not been investigated yet.

The two experimental investigations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite satisfactory.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-bromohexane (1) in water (2) in mass percent, mole fraction, and mole per liter of water given in Table 33 is tentative and based primarily on the reported values of Tewari *et al.*[1] and of Miller *et al.*[2] at 298.15 K.

TABLE 33. Tentative solubility of 1-bromohexane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^6 x_1	$n_1V_2^{-1}$/mol dm^{-3}
25	298.15	0.002 58	2.82	1.56×10^{-4}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromohexane; $C_6H_{13}Br$; [111-25-1] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
25.0	1.56×10^{-4}	2.58×10^{-3}	2.82

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromohexane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector. The result is an average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:
(1) 1-Bromohexane; $C_6H_{13}Br$; [111-25-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Tecnol. **19**, 522 (1985).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
25	0.156	2.58×10^{-3}	2.819

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromohexane. The saturated solution was then pumped through an extractor column and 1-bromohexane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:
(1) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

68. 1-Chlorohexane with Water

Critical Evaluation

The solubility of 1-chlorohexane (1) in water (2) has been studied by two work groups, whereas, the solubility of water (2) in 1-chlorohexane (1) has not been investigated yet.

The two sources of data by Wright and Schaffer[1] and by Leighton and Calo[2] are at different temperatures, so that a direct comparison of the values is not possible. Despite the narrow temperature difference of 2 K, Wright and Schaffer's single value at 298.15 K is about 45% too high. The measurement of Wright and Schaffer[1] is therefore classified as doubtful and it is rejected. The solubility data of Leighton and Calo[2] are believed to be more reliable than the other data because measurements were made at more than one temperature. Leighton and Calo's solubility data were correlated to obtain the following mass percent (1) equation:

$$\text{solubility } [100\ w_1] = -0.019\,959 + 8.852\,89\times10^{-5}\ (T/\text{K}).$$

The above equation represents the smoothed data with a maximum deviation of 17%, usually less, and may be considered tentative for solubilities in the temperature interval from 274 to 296 K. The tentative values for this system in mass percent and mole fraction are given in Table 34 at 5 K intervals.

TABLE 34. Tentative solubility of 1-chlorohexane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^6 x_1
5	278.18	4.67×10^{-3}	6.98
10	283.15	5.11×10^{-3}	7.63
15	288.15	5.55×10^{-3}	8.29
20	293.15	5.99×10^{-3}	8.95
25	298.15	6.43×10^{-3}	9.60

References:

[1] W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
[2] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Components:	**Original Measurements:**
(1) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$V_2g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	1.20×10^4	8.36×10^{-3}	1.25

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1-chlorohexane with a large volume of water and then measuring the volume of the undissolved portion of 1-chlorohexane.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1-Chlorohexane; $C_6H_{13}Cl$; [544-10-5] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=274–296	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^6 x_1 (compiler)
1.00	399.5	3.687×10^{-3}	5.507
3.0	365.5	4.946×10^{-3}	7.387
12.4	668.3	5.645×10^{-3}	8.432
12.5	728.4	5.248×10^{-3}	7.839
17.9	873.2	6.187×10^{-3}	9.241
19.1	969.7	5.929×10^{-3}	8.855
22.7	1161.4	6.237×10^{-3}	9.316
23.0	1267.7	5.783×10^{-3}	8.638

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure

A 5 μL 1-chlorohexane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1-chlorohexane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.8%.
Temperature: ±0.5 K.

Components:	**Evaluator:**
(1) Hexadecafluoroheptane; C_7F_{16}; [335-57-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

69. Hexadecafluoroheptane with Water

Critical Evaluation

The hexadecafluoroheptane (1) and water (2) binary system is treated in two parts; part 1 is hexadecafluoroheptane (1) in water (2) and part 2 is water (2) in hexadecafluoroheptane (1).

Part 1. The solubility of hexadecafluoroheptane (1) in water (2) has been studied by four work groups in the same laboratory, whereas the solubility of water (2) in hexadecafluoroheptane (1) has been reported in one paper only. It is probably safe to assume, the data of Markina *et al.*[1] and of Markina *et al.*[2] have been superseded by those of Kabalnov *et al.*[3] and of Kabal'nov *et al.*,[4] since all four sets of measurements were made in the same laboratory.

The two sets of data, the earlier works of Markina *et al.*[1,2] and the later measurements by Kabalnov *et al.*[3,4] differ substantially by a factor of 4275. However, comparison of the trends in the solubility of perfluorohydrocarbons in water definitely indicate the lower value of Kabalnov *et al.*[3,4] should be preferred. Furthermore, because it is not possible to say which of the two[3,4] is more accurate, it is suggested that the average of the two, which is recorded in Table 35 in mass percent and mole fraction, is probably the most reliable.

TABLE 35. Tentative solubility of hexadecafluoroheptane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^{10} x_1
25	298.15	1.26×10^{-6}	5.84

Part 2. Only the data of Rotariu *et al.*[5] are available for the solubility of water (2) in hexadecafluoroheptane (1); therefore, no critical evaluation is possible. These data are classified as tentative since no other data are available for comparison, see the relevant compilation sheet.

References:

[1] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

[2] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. im. D. I. Mendeleeva **33**, 344 (1988).

[3] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

[4] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

[5] G. J. Rotariu, D. W. Fraga, and J. H. Hildebrand, J. Am. Chem. Soc. **74**, 5783 (1952).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Hexadecafluoroheptane; C_7F_{16}; [335-57-9]	G. J. Rotariu, D. W. Fraga, and J. H. Hildebrand, J. Am. Chem. Soc. **74**, 5783 (1952).
Variables:	**Prepared By:**
T/K=298–323	A. L. Horvath

Experimental Data

t/°C	100 V_1 /V	100 w_1	10^4 x_1 (compiler)
25	3.7×10^{-3}	2.2×10^{-3}	4.74
50	9.3×10^{-3}	5.4×10^{-3}	11.6

Auxiliary Information

Method/Apparatus/Procedure:

The solute–solvent mixture was rocked for 24 h in a waterbath thermostat. Samples were removed from the organic rich phase with a special pipet with a turned up tip. During the removal and the analysis with the Karl Fischer reagent, the liquid was exposed only to dry nitrogen. The result is the mean value of five determinations.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source not given. Purified in a silicagel column followed by distillation. Sample contained 0.1% hydrocarbon.

Estimated Errors:

Solubility: ±30%.
Temperature: ±0.01 K.

Components:

(1) Hexadecafluoroheptane; C_7F_{16}; [335-57-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ x_1$	c_1 /mol dm^{-3}	$100\ w_1$
19.85	2.6	1.45×10^{-4}	5.6×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of hexadecafluoroheptane in water was determined through the use of precision tensiometric measurements for aqueous solutions of perfluorononane acid on its interface with perfluorodecalin at 293 K. The measurements served as a basis for evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from the water phase into a perfluoroorganic liquid phase.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

Components:

(1) Hexadecafluoroheptane; C_7F_{16}; [335-57-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. im. D. I. Mendeleeva **33**, 344 (1988).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ x_1$	c_1 /mol dm^{-3}	$100\ w_1$
20	2.6	1.45×10^{-4}	5.6×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The colloid chemical method was used for observing the shift in the critical micelle concentration formation for a surfactant in aqueous solutions under the influence of halogenated hydrocarbons. The solubility was calculated from the increment of standard chemical potential for the transfer of a fluoromethylene group from water into the fluorocarbon phase on the basis of experimental determination of the surface activity of a perfluoroorganic surface active nonelectrolyte.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Hexadecafluoroheptane; C_7F_{16}; [335-57-9] (2) Water; H_2O; [7732-18-5]	A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
2.5	3.1×10^{-8}	1.20×10^{-6}	5.58

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial grade, >99% pure.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1.0 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:	**Original Measurements:**
(1) Hexadecafluoroheptane; C_7F_{16}; [335-57-9] (2) Water; H_2O; [7732-18-5]	A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^{10} x_1 (compiler)
25	7.56×10^{-7}	1.31×10^{-6}	6.098

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of hexadecafluoroheptane in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of the coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent, >99% pure, passed through a column with Al_2O_3 before use.
(2) Double distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:	**Evaluator:**
(1) 1-Bromoheptane; $C_7H_{15}Br$; [629-04-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993

70. 1-Bromoheptane with Water

Critical Evaluation

The solubility of 1-bromoheptane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1-bromoheptane (1) has not been investigated yet.

The two experimental investigations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite satisfactory.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-bromoheptane (1) in water (2) given in Table 36 in mass percent, mole fraction, and mole per liter of water is tentative and based primarily on the reported values of Tewari *et al.*[1] and of Miller *et al.*[2] at 298.15 K.

TABLE 36. Tentative solubility of 1-bromoheptane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^7\ x_1$	$n_1V_2^{-1}$/mol dm^{-3}
25	298.15	6.68×10^{-4}	6.72	3.71×10^{-5}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromoheptane; $C_7H_{15}Br$; [629-04-9] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data. **27**, 451 (1982).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	$10^7\ x_1$ (compiler)
25.0	3.71×10^{-5}	6.68×10^{-4}	6.72

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromoheptane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector. The results is the average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:

(1) 1-Bromoheptane; $C_7H_{15}Br$; [629-04-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:

$T/\mathrm{K}=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	$n_1V_2^{-1}/\mathrm{mol\ m}^{-3}$	$100\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
25.0	3.71×10^{-2}	6.68×10^{-4}	6.72

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromoheptane. The saturated solution was then pumped through an extractor column and 1-bromoheptane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1.0 K (compiler).

Components:

(1) 1-Chloroheptane; $C_7H_{15}Cl$; [629-06-1]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

71. 1-Chloroheptane with Water

Critical Evaluation

The solubility of 1-chloroheptane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1-chloroheptane (1) has not been investigated yet.

The two experimental investigations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite reliable.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-chloroheptane (1) in water (2) given in Table 37 in mass percent, mole fraction, and mole per liter of water is tentative and based primarily on the reported value of Tewari *et al.*[1] and of Miller *et al.*[2] at 298.15 K.

TABLE 37. Tentative solubility of 1-chloroheptane (1) in water (2)

Temperature		Solubility		
°C	K	$100\ w_1$	$10^6\ x_1$	$n_1V_2^{-1}/\mathrm{mol\ dm}^{-3}$
25	298.15	1.36×10^{-3}	1.82	1.01×10^{-4}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Chloroheptane; $C_7H_{15}Cl$; [629-06-1] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
25.0	1.01×10^{-4}	1.36×10^{-3}	1.82

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-chloroheptane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector. The result is an average of at last three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%
Temperature: ±1.0 K.

Components:	**Original Measurements:**
(1) 1-Chloroheptane; $C_7H_{15}Cl$; [629-06-1] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
25	0.101	1.36×10^{-3}	1.82

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-chloroheptane. The saturated solution was then pumped through an extractor column and 1-chloroheptane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Evaluator:**
(1) 1-Iodoheptane; $C_7H_{15}I$; [4282-40-0] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries, Limited, Runcorn, U.K., July 1993.

72. 1-Iodoheptane with Water

Critical Evaluation

The solubility of 1-iodoheptane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1-iodoheptane (1) has not been investigated yet.

The two experimental investigations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite reliable.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-iodoheptane (1) in water (2) given in Table 38 in mass percent, mole fraction, and mole per liter of water is tentative and based primarily on the reported value of Tewari *et al.*[1] and Miller *et al.*[2] at 298.15 K.

TABLE 38. Tentative solubility of 1-iodoheptane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^7 x_1	$n_1V_2^{-1}$/mol dm^{-3}
25	298.15	3.50×10^{-4}	2.80	1.55×10^{-5}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Iodoheptane; $C_7H_{15}I$; [4282-40-0] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^7 x_1 (compiler)
25.0	1.55×10^{-5}	3.50×10^{-4}	2.80

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-iodoheptane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector. The result is an average of at least three measurements.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:
(1) 1-Iodoheptane; $C_7H_{15}I$; [4282-40-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^7 x_1 (compiler)
25	1.55×10^{-2}	3.50×10^{-4}	2.80

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-iodoheptane. The saturated solution was then pumped through an extractor column and 1-iodoheptane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:
(1) Octadecafluorooctane; C_8F_{18}; [307-34-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

73. Octadecafluorooctane with Water

Critical Evaluation

The solubility of octadecafluorooctane (1) in water (2) has been studied by four work groups in the same laboratory, whereas the solubility of water (2) in octadecafluorooctane (1) has not been investigated yet.

It is probably safe to assume the data of Markina *et al.*[1] and of Markina *et al.*[2] have been superseded by those of Kabalnov *et al.*[3] and of Kabal'nov *et al.*,[4] since all four sets of measurements were made in the same laboratory.

The two sets of data, the earlier works of Markina *et al.*[1,2] and the later measurements by Kabalnov *et al.*[3,4] differ substantially by a factor of 5848. However, comparison of the trends in the solubility of perfluorohydrocarbons in water (see Preface) definitely indicate the lower value of Kabalnov *et al.*[3,4] should be preferred. Furthermore, because it is not possible to say which of the two[3,4] is more accurate, it is suggested that the average of the two, which is recorded in Table 39 in mass percent, mole fraction, and mole per 100 g, is probably the most reliable.

TABLE 39. Tentative solubility of octadecafluorooctane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^{11} x_1	100 $w_1M_1^{-1}$/mol g^{-1}
25	298.15	1.71×10^{-7}	7.06	3.90×10^{-10}

References:

[1] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

[2] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. Im. D. I. Mendeleeva **33**, 344 (1988).

[3] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

[4] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

Components:

(1) Octadecafluorooctane; C_8F_{18}; [307-34-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^7\ x_1$	c_1 /mol dm^{-3}	100 w_1
19.85	4.15	2.3×10^{-5}	1.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of octadecafluorooctane in water was determined through the use of precision tensiometric measurements for aqueous solutions of perfluorononane acid on its interface with perfluorodecalin at 293 K. The measurements served as a basis for evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from the water phase into a perfluoroorganic liquid phase.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Octadecafluorooctane; C_8F_{18}; [307-34-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Z. N. Markina, N. M. Zadymova, E. D. Shukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-Va. im. D. I. Mendeleeva **33**, 344 (1988).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^7\ x_1$	c_1 /mol dm^{-3}	100 w_1
20	4.15	2.3×10^{-5}	1.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The colloid chemical method was used for observing the shift in the critical micelle concentration formation for a surfactant in aqueous solutions under the influence of halogenated hydrocarbons. The solubility was calculated from the increment of standard chemical potential for the transfer of a fluoromethylene group from water into the fluorocarbon phase on the basis of experimental determination of the surface activity of a perfluoroorganic surface active nonelectrolyte.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Octadecafluorooctane; C_8F_{18}; [307-34-6] (2) Water; H_2O; [7732-18-5]	A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^{11} x_1 (compiler)
25	3.8×10^{-9}	1.66×10^{-7}	6.85

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial grade, >99% pure.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1.0 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:	**Original Measurements:**
(1) Octadecafluorooctane; C_8F_{18}; [307-34-6] (2) Water; H_2O; [7732-18-5]	A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^{11} x_1 (compiler)
25	1.02×10^{-7}	1.77×10^{-7}	7.28

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of octadecafluorooctane in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of the coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent, >99% pure, passed through a column with Al_2O_3 before use.
(2) Double distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:	**Evaluator:**
(1) 1-Bromooctane; $C_8H_{17}Br$; [111-83-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

74. 1-Bromooctane with Water

Critical Evaluation

The solubility of 1-bromooctane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1-bromooctane (1) has not been investigated yet.

The two experimental investigations by Tewari *et al.*[1] in 1982 and by Miller *et al.*[2] in 1985 are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved a modified generator column procedure, gives relatively accurate results. Upon consideration of saturation equilibrium, the method of analysis, and the reported standard deviation, one may conclude the solubility value is quite satisfactory.

There are not enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative. The following solubility of 1-bromooctane (1) in water (2) given in Table 40 in mass percent, mole fraction, and mole per liter water is tentative and based primarily on the reported value of Tewari *et al.*[1] and of Miller *et al.*[2] at 298.15 K.

TABLE 40. Tentative solubility of 1-bromooctane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^7 x_1	$n_1V_2^{-1}$/mol dm^{-3}
25	298.15	1.67×10^{-4}	1.56	8.65×10^{-6}

References:

[1] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[2] M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Components:	**Original Measurements:**
(1) 1-Bromooctane; $C_8H_{17}Br$; [111-83-1] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^7 x_1 (compiler)
25.0	8.65×10^{-6}	1.67×10^{-4}	1.56

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid 1-bromooctane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a gas chromatographic method using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

Components:

(1) 1-Bromooctane; $C_8H_{17}Br$; [111-83-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^7 x_1 (compiler)
25	8.65×10^{-3}	1.67×10^{-4}	1.56

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with 1-bromooctane. The saturated solution was then pumped through an extractor column and 1-bromooctane was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both a UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Company. Commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1-Chlorooctane; $C_8H_{17}Cl$; [111-85-3]

Original Measurements:

A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, 1938, 159 pp.

Variables:

T/K=298

Prepared By:

A. L. Horvath

75. 1-Chlorooctane with Water

Experimental Data

t/°C	100 w_1	10^3 x_1	10 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	3.45×10^{-2}	2.85	1.915×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with 1-chlorooctane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate.

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,1,2,2,3,4,5,5,5-Decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane; C_9F_{20}; [50285-18-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

76. 1,1,1,2,2,3,4,5,5,5-Decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane with Water

Critical Evaluation

The solubility of 1,1,1,2,2,3,4,5,5,5-decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in 1,1,1,2,2,3,4,5,5,5-decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane (1) has not been investigated yet.

In both the experiments of Kabal'nov *et al.*[1] and of Kabalnov *et al.*[2] the solubility was calculated from the particle size growth in emulsions due to Ostwald ripening at 298.15 K. The reported data are in reasonable agreement with respect to the errors estimated by the authors.

It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to have produced relatively accurate results. When one considers the saturation equilibrium, the method of analysis, and the reported standard deviation, one can conclude the values are reasonably accurate. Because it is not possible to say which of the two data points of Kabal'nov *et al.*[1] and of Kabalnov *et al.*[2] is more accurate, it is suggested that the average of the two as presented in Table 41 in mass percent, mole fraction, and mole per 100 g is possibly the most reliable.

TABLE 41. Tentative solubility of 1,1,1,2,2,3,4,5,5,5-decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(tetrafluoromethyl)pentane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^{11}\ x_1$	100 $w_1M_1^{-1}$/mol g^{-}
25	298.15	1.27×10^{-7}	4.68	2.60×10^{-10}

References:

[1] A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

[2] A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

Components:

(1) 1,1,1,2,2,3,4,5,5,5-Decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane; C_9F_{20}; [50285-18-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Kabal'nov, L. D. Gervits, and K. N. Makarov, Kolloidnyi Zh. **52**, 1060 (1990).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	$10^{11}\ x_1$ (compiler)
25	6.86×10^{-8}	1.317×10^{-7}	4.86

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of the fluorocarbon in water was calculated from the kinetic data derived from observations of particle growth in aqueous emulsions in which Ostwald ripening takes place. The kinetics of coarsening of particles was observed by photon correlation spectroscopy on a Coulter N4 instrument. The calculation was based upon the Lifshits–Slezov equation.

Source and Purity of Materials:

(1) Commercial reagent. 97% pure, passed through a column with Al_2O_3 before use.
(2) Double distilled and de-ionized.

Estimated Errors:

Solubility: Twice that of other results.
Temperature: ±1 K.

Components:	**Original Measurements:**
(1) 1,1,1,2,2,3,4,5,5,5-Decafluoro-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-4-(trifluoromethyl)pentane; C_9F_{20}; [50285-18-2] (2) Water; H_2O; [7732-18-5]	A. S. Kabalnov, K. N. Makarov, and O. V. Shcherbakova, J. Fluorine Chem. **50**, 271 (1990).

Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	c_1 /mol dm^{-3}	100 w_1 (compiler)	10^{11} x_1 (compiler)
25	2.5×10^{-9}	1.22×10^{-7}	4.50

Auxiliary Information

Method/Apparatus/Procedure:

The solubility values were calculated from the particle size growth in emulsions due to Ostwald ripening. The particle size analysis of emulsions was accomplished through the use of a photon correlation spectrometer. The kinetics of particle size growth were observed until a 200 nm diameter was attained. The solubility measurement method showed a very low detection limit. Further details on Ostwald ripening kinetics are described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial grade, 97% pure.
(2) Doubly distilled and de-ionized.

Estimated Errors:

Solubility: About ±30%.
Temperature: ±1.0 K.

References:

[1] P. W. Voorhees, J. Stat. Phys. **38**, 231 (1985).

Components:	**Original Measurements:**
(1) Docosafluorodecane; $C_{10}F_{22}$; [307-45-9] (2) Water; H_2O; [7732-18-5]	Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidn. Zh. **49**, 1084 (1987).

Variables:	**Prepared By:**
T/K=293	A. L. Horvath

77. Docosafluorodecane with Water

Experimental Data

t/°C	10^8 x_1	c_1 /mol dm^{-3}	100 w_1
19.85	1.05	5.8×10^{-7}	3.1×10^{-5}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of docosafluorodecane in water was determined through the use of precision tensiometric measurements for aqueous solutions of perfluorononane acid on its interface with perfluorodecalin at 293 K. The measurements served as a basis for evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from the water phase into a perfluoroorganic liquid phase.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

Components:	**Evaluator:**
(1) Hexacosafluorododecane; $C_{12}F_{26}$; [307-59-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., July 1993.

78. Hexacosafluorododecane with Water

Critical Evaluation

The solubility of hexacosafluorododecane (1) in water (2) has been studied by two work groups in the same laboratory, whereas the solubility of water (2) in hexacosafluorododecane (1) has not been investigated yet.

The two experimental investigations by Markina *et al.*[1] and by Markina *et al.*[2] are in excellent agreement with respect to the errors estimated by the authors. It is not possible to establish any shortcomings of the experimental procedures from the description. The measurements seem to be performed with care and the method, which involved the evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from water into a perfluoroorganic liquid, gives relatively acceptable results.

There are not enough measurements to allow a more rigorous evaluation to be made; therefore, the solubility values reported here must be tentative. The following solubility of hexacosafluorododecane (1) in water (2) given in Table 42 in mass percent, mole fraction, and mole per liter water is tentative and based primarily on the reported value of Markina *et al.*[1] and of Markina *et al.*[2] at 293.15 K.

TABLE 42. Tentative solubility of hexacosafluorododecane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^{10} x_1	$n_1V_2^{-1}$/mol dm^{-3}
20	293.15	9.6×10^{-7}	2.7	1.5×10^{-8}

References:

[1] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).

[2] Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-va. im. D. I. Mendeleeva **33**, 344 (1988).

Components:	**Original Measurements:**
(1) Hexacosafluorododecane; $C_{12}F_{26}$; [307-59-5] (2) Water; H_2O; [7732-18-5]	Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Kolloidnyi Zh. **49**, 1084 (1987).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	10^{10} x_1	c_1 /mol dm^{-3}	100 w_1
19.85	2.7	1.5×10^{-8}	9.6×10^{-7}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of hexacosafluorododecane in water was determined through the use of precision tensiometric measurements for aqueous solutions of perfluorononane acid on its interface with perfluorodecalin at 293 K. The measurements served as a basis for evaluation of the increment of the standard chemical potential for the transition of a perfluoromethylene group from the water phase into a perfluoroorganic liquid phase.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Hexacosafluorododecane; $C_{12}F_{26}$; [307-59-5] (2) Water; H_2O; [7732-18-5]	Z. N. Markina, N. M. Zadymova, E. D. Shchukin, K. N. Makarov, and L. L. Gervits, Zh. Vses. Khim. O-va. im. D. I. Mendeleeva **33**, 344 (1988).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^{10}\ x_1$	c_1 /mol dm^{-3}	100 w_1
20	2.7	1.5×10^{-8}	9.6×10^{-7}

Auxiliary Information

Method/Apparatus/Procedure:

The colloid chemical method was used for observing the shift in the critical micelle concentration formation for a surfactant in aqueous solutions under the influence of halogenated hydrocarbons. The solubility was calculated from the increment of standard chemical potential for the transfer of a fluoromethylene group from water into the fluorocarbon phase on the basis of experimental determination of the surface activity of a perfluoroorganic surface active nonelectrolyte.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1-Chlorotetradecane; $C_{14}H_{29}Cl$; [2425-54-9]	A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, 1938, 159 pp.
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

79. 1-Chlorotetradecane with Water

Experimental Data

t/°C	100 w_1	$10^3\ x_1$	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	2.32×10^{-2}	3.28	1.29×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with 1-chlorotetradecane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. A full description of the method used is given in the doctoral dissertation.

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.5 K (compiler).

80. System Index

Page numbers preceded by E refer to evaluation texts, whereas those not preceded by E refer to compiled tables. Substances are listed in the Chemical Abstracts.

81. Registry Number Index

Page numbers preceded by E refer to evaluation texts, whereas those not preceded by E refer to compiled tables.

82. Author Index

Pages preceded by an E refer to evaluation texts, whereas those not preceded by E refer to compiled tables.