# IUPAC-NIST Solubility Data Series. 77. $C_{2+}$ Nitroalkanes With Water or Organic Solvents: Binary and Multicomponent Systems

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The mutual solubilities and liquid-liquid equilibria of binary and multicomponent systems composed of $C_{2+}$ nitroalkanes with solvents are reviewed. The solvents (mainly in liquid phase) include water, inorganic compounds and a variety of organic compounds such as hydrocarbons, halogenated hydrocarbons, alcohols, acids, esters, and nitrogen compounds. A total 81 binary, 21 ternary, 2 quaternary and 1 five component systems whose properties were described in the chemical literature through 1998 are compiled. For 14 systems sufficient data were available to allow critical evaluation. All data are expressed as mass and mole fractions as well as the originally reported units. Similar reviews of gas, liquid and solid solubilities for other systems have been within the Solubility Data Series. This is volume 77 of this series. © *2002 American Institute of Physics.*

Key words: aqueous solution; binary systems; liquid–liquid equilibrium; nitroethane; 1-nitropropane; 2-nitropropane; 2-nitrobutane; organic solvents; pentacomponent systems; quaternary systems; solubility; ternary systems.

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# 1. Preface

## 1.1. Scope of the Volume

This volume reviews experimentally determined solubility data for well defined binary and multicomponent systems in which one component is nitroalkane (nitroethane, 1-nitropropane, 2-nitropropane, nitrobutanes). Other components for which data were found in the chemical literature include water, organic substances of various classes (hydrocarbons of several structural types, halogenated hydrocarbons, mono and polyhydroxy alcohols, acids, ethers, esters) and inorganic substances. An exhaustive search of the chemical literature published prior to 1998 found solubility data for 81 binary, 21 ternary, 2 quaternary, and 1 five component systems. From these, 144 Compilations were prepared. Most Compilations present the solubility data for one system as reported in one publication. For some original publications, which report very limited data for several systems, those data are grouped into a single Compilation. Where two or more reliable Compilations were found for a system, a Critical Evaluation was prepared. This was possible for only 14 systems, reflecting the sparseness of study of many nitroalkane systems. The systems are ordered on the basis of the chemical formula according to the Hill system (described in the Introduction), except for those Compilations where more than one system is treated.

To the extent allowed by the available data, this volume considers mutual solubility and liquid–liquid equilibrium of binary and multicomponent systems. That is, data for both the solubility of nitroalkane in other components and the solubility of the components in nitroalkane are compiled and evaluated when available. Other solubility data, which are compiled when available, include the distribution of *i* component between coexistent liquid phases of ternary systems. Numerical data reported in the primary sources were used for preparation of compilations. When data were presented only in graphical form, the compilers attempted to obtain numerical data from the original investigators. In some cases where numerical data could not be obtained in this way, the compilers extracted the numerical data from published diagrams.

This volume is the result of an exhaustive search of the chemical literature using both Chemical Abstracts and Russian Abstract Journal for Chemistry (Referativnyi Zhurnal ''Khimiya''). The goal of the search was to include all published data for systems designated in the title. Russian archival sources including Deposited Documents of VINITI, scientific works (Nauchnye Trudy or Uchenye Zapiski) of Universities, Research Institutes and Educational Institutions, and materials from conferences, meetings, and symposia are also included. Each critical evaluation includes the date at which the literature search closed for the system evaluated (usually 1998). In spite of all efforts, some sources of experimental data may have been missed. The editors will gratefully receive information about omissions.

In some original sources solubility data is reported as incidental or ancillary information to other studies. If, for this or other reasons, details concerning experimental methods, source and purity of materials, or estimated errors are brief or absent, correspondingly short entries appear in the compilations, sometimes with the note, ''No further details were reported.'' Estimated errors were sometimes provided by the compiler with appropriate notation.

For convenience of comparison of experimental data, compilers and the evaluator of this volume, in so far as is possible, expressed all initial results in mass percent and mole fraction as well as in units reported in the original source. Conversions, where they were made, are clearly attributed to the compiler. Some unit conversions require numerical data for the density of pure components and/or the mixtures. Approximate values of mixture densities obtained using calculations recommended in standard handbooks, for example Reid, *et al.*[1] Definitions of mass percent and mole fraction as well as their relation to other units of solubility are given in the Introduction.

The solubility data, for the particular system in which UCST (Upper Critical Solubility Temperature) appears, could be described by the equation based on the scaling law with the corrections terms. This equation has been also discussed in detail by Lorimer, *et al.*[2] And it has the form as in Wegner:[3]

$$x_1 = x_{c1} + b_1 \cdot \Theta + b_2 \cdot \Theta^{1-\alpha} + b_3 \cdot \Theta^{1-\alpha+\omega} \pm a_1 \cdot \Theta^{\beta} \pm a_2 \cdot \Theta^{\beta+\omega} \pm a_3 \cdot \Theta^{\beta+2\omega} \quad (1)$$

where

$$\Theta = (T_c - T)/T_c. \quad (2)$$

The $a_i$, $b_i$ are the adjustable parameters. According to the above literature, the equation factors are assumed to be:

$$\beta = 0.329; \quad \alpha = 0.11; \quad \omega = 0.5.$$

The equation is valid usually when $(T_c - T)/T_c > 10^{-3}$, which in the discussed systems is equivalent to the temperature range of about 0.3–0.4 K below the UCST. For the systems discussed further in the evaluation tables the equation was used generally in the simplified version without $b_3$ and $a_3$ elements.

The general properties of ternary systems exhibiting liquid–liquid equilibrium and basic types of the solubility curves have been treated in detail.[4] Ternary systems with limited mutual solubility of components representing interest for liquid extraction, have been classified by Treybal[4] as follows:

Type I. Systems with one pair partially miscible liquids.

Type II. Systems with two pairs of partially miscible liquids.

Type III. Systems with three pairs of partially miscible liquids.

Type IV. Systems forming solid phases.

In this volume 6 systems, 29%, are Type I.

In the series of ternary systems nitroethane +1-normal alcohols+water $C_3$ alcohols are Type I. Depending on temperature systems with $C_9$–$C_{12}$ alcohols can correspond to Type I–IV. For example, the system nitroethane +1-nonanol +water at temperatures below 287 K has three pairs of partially soluble liquids and falls into Type III. In the temperature interval 287–443.5 K, where the two binary pairs nitroethane+water and 1-nonanol+water are partially soluble, the ternary system is Type II. Above 443.5 K this ternary system is Type I. Three fluid phases are present in the temperature interval 273–278 K.

### 1.2. Experimental Methods

Most solubility measurements of binary and multicomponent systems containing nitroalkanes have been made between room temperature and the UCST (upper critical solution temperature) of the binary system under study. At atmospheric pressure temperatures studied range from 230 K (Nitroethane+1-Hexene) to 472 K (Nitroethane+1-Dodecanol+Water). Three basic approaches to solubility measurement for binary and multicomponent systems are known: synthetic, titration and analytical. Of these the synthetic (visual-polythermal, or cloud-point) method is most commonly used. Almost 76% (110) of the compilations in this volume are for data obtained using the synthetic method. In this method the temperature is determined at which turbidity associated with a second phase appears and/or disappears for a mixture of known composition, often in a sealed ampoule. In some systems the ternary or multicomponent mixtures form three or four fluid phases. In these cases continued heating determines first the temperature of dissolution of the third fluid phase (solubility temperature of the three liquid phases), and then at higher temperature dissolution of the second fluid phase (solubility temperature of the two liquid phases).

This method was introduced by Alekseev[5] (also transliterated in some older German language publications as ''Alexeev'' or ''Alexejew'') in 1876. The method has been refined and improved by Rothmund,[6] and by Timmermans[7] and is capable of measuring solution temperature with an error (±0.01 K). System pressure at the solution temperature is seldom reported since it is assumed that the effect of pressure is minor.

Two other methods are used for isothermal measurements of solubility. In the titration method one component is added in small portions with vigorous mixing to a solution of the remaining components until persistent turbidity is observed. In the analytical method samples of liquid phases at equilibrium are analyzed by various methods: chemical or physical. Sources of error in these three methods include gravitational effects and impurities in materials whose solubilities are being determined. This has been discussed in detail.[2] For ternary mixtures of nitroalkane and organic substances, water is a common impurity since it is difficult to remove completely from most organic liquids and is reabsorbed on exposure to air. The presence of small quantities of water can either lower the temperature of solubility (e.g., in systems of nitroalkane and alcohols) or raise these temperatures (e.g., in mixtures of nitroalkane and hydrocarbons).[8]

### 1.3. Procedure Used in Critical Evaluations

A Critical Evaluation was prepared for each system for which two or more independent reports of solubility are available. In evaluating the available data the evaluators have considered both the data quality of individual original sources to the extent that can be established from the content (and omissions) of those reports and by comparing the results obtained independently in more than one laboratory. Several aspects of the solubility data have been considered: purity of substances and date of experiment; accuracy of the method and reproducibility of the experiment; experience of the researcher(s) and previous publications.

In Critical Evaluations data may be classified as *Recommended*, *Tentative*, or *Rejected*. Data are recommended if the results of two or more independent groups are in good agreement and the evaluator has no doubt of the adequacy of the experimental and computational procedures used. Data are classified as tentative if only one set of measurements is available or if the evaluator considers some aspect of the experimental or computational procedures as mildly questionable. Data determined by an inadequate or ill-defined method are rejected. Where it is possible, Recommended or Tentative values of mutual solubility and liquid–liquid equilibrium, are specified at 0.1 MPa. Solubility data at several temperatures are described by an algebraic equation (1).

The equation parameters are presented in Critical Evaluations and were calculated by the least squares method so that the smoothing equation gives smaller standard deviations

than any other tested equations. The solubilities calculated by the proposed equation are presented in the figures and tables. Experimental solubility data from references are presented in figures for comparison.

Graphical representations of all reported data are often useful for comparing data and identifying outliers and are included in some Evaluations. These diagrams, representing the solubility data and the compositions of coexisting liquid phases at several temperatures (expressed in mole fraction) can reveal whether or not a trend exists among the data in addition to highlighting any discrepancies of experimental solubility measurements.

The editors wish to acknowledge with thanks the help of Professor I. A. Dibrov (Russia) who provided copies of several of the articles reviewed in this volume and also Rector of the Samarian Technical University Professor Yu. P. Samarin for support and help for preparation of this volume.

### 1.4. References for the Preface

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

### 2.1. The 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 independent 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 or 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-l-butene |
| | 2-methyl-2-butene |
| | 1-pentene |
| | 2-pentene |
| $C_5H_{12}$ | 2,2-dimethylpropane |
| | 2-methylbutane |
| | pentane |
| $C_5H_{12}O$ | 2,2-dimethyl-l-propanol |
| | 2-methyl-l-butanol |
| | 2-methyl-2-butanol |
| | 3-methyl-l-butanol |
| | 3-methyl-2-butanol |
| | 1-pentanol |
| | 2-pentanol |
| | 3-pentanol |
| $C_6H_{12}O$ | cyclohexanol |
| | 4-methyl-l-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 indicated 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 Data

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 an 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, as 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 estimated 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 fraction 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 form 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, IUPAC Green Book.[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) (condensed phases), $y_1$ (gases):

$$x_1 = n_1 \Big/ \sum_{s=1}^{c} n_s \tag{1}$$

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 100 $x_1$.

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 $v_{s+}$ cations and $v_{s-}$ anions, with $v_s = v_{s+} + v_{s-}$ and a mixture of $p$ nonelectrolytes $j$, of which some may be solvent components, a generalization of the definition in Ref. 11 gives

$$x_{i+} = \frac{v_i + x_i}{1 + \sum_{i=1}^{s} (v_i - 1) x_s}, \quad x_{i-} = \frac{v_{i-} x_{i+}}{v_{i+}} \quad i = 1 \ldots s \tag{2}$$

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

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,

$$x_1 = \frac{v_{2+} x'_1}{v_{2+} - (v_2 - 1) x_{2+}}, \quad x_2 = \frac{x_{2+}}{v_{2+} - (v_2 - 1) x_{2+}}. \tag{5}$$

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 $w(1)$:

$$w_1 = g_1 \Big/ \sum_{s=1}^{c} g_s \tag{6}$$

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

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

$$m_1 = n_1 / n_2 M_2 \tag{7}$$

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] $m_1^{(3)}$:

$$m_1^{(3)} = m_1 \overline{M} / M_3 \tag{8}$$

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

$$\overline{M} = x'_2 M_2 + (1 - x'_2) M_3 \tag{9}$$

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* if 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 $V$, SI $\rho_1$: 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*, $\rho$:

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

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

10. *Relative density*, $d = \rho / \rho^\circ$: the ratio of the density of a mixture at temperature $t$, pressure $p$ to the density of a reference 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 aims are often difficult to achieve because of a

TABLE 1. Interconversions between quantities used as measures of solubilities $c$-component systems containing $c$-1 solutes $i$ and single solvent $c$ ($\rho$—density of solution; $M_i$—molar masses of $i$. For relations for two-component systems, set summations to 0.)

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

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 this 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 (1980).

[3] I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry* (The Green Book). (Blackwell Scientific Publications, 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 (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 Publications, Oxford, UK, 1987).

[7] H. Freiser and G. H. Nancollas, eds., *Compendium of Analytical Nomenclature* (The Orange Book) (The Blackwell Scientific Publications, 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 Verlag, Berlin, 1984).

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

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

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



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December, 1995

# 3. Nitroethane: Binary Systems

## 3.1. Water

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

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

Table 1. Summary of solubility data for the system nitroethane+water

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Malone and Vining[1] | 298 | mutual | titration |
| Tolstova and Sheblom[2] | 293 | mutual | titration |
| Zhuravleva *et al.*[3] | 295 to 444 | mutual | synthetic |
| Hampe[4] | 293 | mutual | not stated |
| Stephenson[5] | 273 to 364 | mutual | not stated |

All original data are compiled in the data sheets immediately following this Critical Evaluation. The water-rich phase data of Malone and Vining[1] at 298 K and nitroethane-rich phase data of Tolstova and Sheblom[2] at 293 K disagree markedly from all other studies and are rejected. All other reported data are included in Tables 2 and 3.

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

Table 2. Tentative and recommended (R) values for the solubility nitroethane (1) in water (2)

| $T$/K | Solubility, 100 $w_1$ Reported values | "Best" values ($\pm\sigma_n$) 100 $w_1$ | $x_1$ |
|---|---|---|---|
| 273.2 | 4.32 (Ref. 5) | 4.32 | 0.0107 |
| 283.2 | 4.2*(Ref. 5) | 4.2 | 0.010 |
| 293.2 | 4.5 (Ref. 2), 4.68 (Ref. 4), 4.4*(Ref. 5) | 4.5±0.1 (R) | 0.011 |
| 298.2 | 4.4*(Ref. 3), 4.4*(Ref. 5) | 4.4 (R) | 0.011 |
| 303.2 | 4.5 (Ref. 3), 4.4*(Ref. 5) | 4.45±0.05(R) | 0.0111 |
| 313.2 | 4.9*(Ref. 3), 4.6*(Ref. 5) | 4.75±0.2 (R) | 0.0118 |
| 323.2 | 5.5 (Ref. 3), 5.1*(Ref. 5) | 5.3±0.2 (R) | 0.013 |
| 333.2 | 6.2*(Ref. 3), 5.4*(Ref. 5) | 5.8±0.4 | 0.015 |
| 343.2 | 6.9*(Ref. 3), 5.8*(Ref. 5) | 6.4±0.5 | 0.016 |
| 353.2 | 8.8*(Ref. 3), 6.2*(Ref. 5) | 7.5±1.3 | 0.019 |
| 363.2 | 10.8*(Ref. 3), 6.6*(Ref. 5) | 8.7±2 | 0.022 |
| 373.2 | 12.9*(Ref. 3) | 12.9 | 0.0343 |
| 393.2 | 16.9*(Ref. 3) | 16.9 | 0.0465 |
| 413.2 | 23.0*(Ref. 3) | 23.0 | 0.0669 |
| 433.2 | 35.0 (Ref. 3) | 35.0 | 0.115 |
| 443.2 | 52.5*(Ref. 3) | 52.5 | 0.210 |

Table 3. Tentative and recommended (R) values for the solubility water (2) in nitroethane (1)

| $T$/K | Solubility, 100 $w_2$ Reported values | "Best" values ($\pm\sigma_n$) 100 $w_2$ | $x_2$ |
|---|---|---|---|
| 273.2 | 0.62 (Ref. 5) | 0.62 | 0.025 |
| 283.2 | 0.8*(Ref. 5) | 0.8 | 0.033 |
| 293.2 | 1.05 (Ref. 4), 1.0*(Ref. 5) | 1.0 (R) | 0.040 |
| 298.2 | 0.86 (Ref. 1), 0.9*(Ref. 3), 1.15*(Ref. 5) | 1.0±0.1 | 0.040 |
| 303.2 | 1.1 (Ref. 9), 1.3*(Ref. 5) | 1.2±0.1 | 0.048 |
| 313.2 | 1.4*(Ref. 3), 1.6*(Ref. 5) | 1.5±0.1 | 0.060 |
| 323.2 | 1.8*(Ref. 3), 1.9*(Ref. 5) | 1.85±0.05(R) | 0.0728 |
| 333.2 | 2.1*(Ref. 3), 3.2*(Ref. 5) | 2.7±0.6 | 0.104 |
| 343.2 | 2.9*(Ref. 3), 4.7*(Ref. 5) | 3.8±0.9 | 0.141 |
| 353.2 | 4.0 (Ref. 3), 6.1*(Ref. 5) | 5.0±1 | 0.180 |
| 363.2 | 6.3*(Ref. 3), 7.1*(Ref. 5) | 6.7±0.4 | 0.230 |
| 373.2 | 8.4*(Ref. 3) | 8.4 | 0.276 |
| 393.2 | 12.6*(Ref. 3) | 12.6 | 0.375 |
| 413.2 | 17.1*(Ref. 3) | 17.1 | 0.462 |
| 433.2 | 24.3*(Ref. 3) | 24.3 | 0.572 |
| 443.2 | 42.5*(Ref. 3) | 42.5 | 0.755 |

The interpolated values reported in the tables above were approximated using an equation based on the scaling law (described in the preface) for which following parameters were derived:

$$a_1=0.50432,\quad a_2=0.30838,\quad b_1=-2.72914,\quad b_2=3.07370 \text{ (mean standard error of estimate was 0.0288).}$$

For this approximation the values of UCST and $x_{c1}$ from Zhuravleva, *et al.*[3] have been used. The calculated compositions are within the stated accuracy of the tables at each point. The calculated relationship is presented in Fig. 1 together with the "best" values from the above tables.

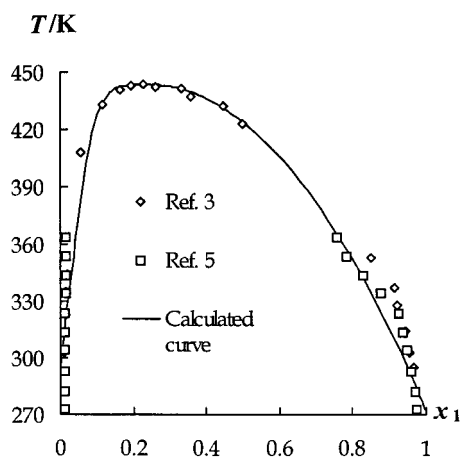


FIG. 1. Mutual solubility of nitroethane and water.

The upper critical solution temperature was reported to be 443.7 K.[3] The corresponding critical solution composition was reported to be $x_{c1}=0.227$.[3] These values are tentative.

**References:**

[1]J. W. Malone and R. W. Vining, J. Chem. Eng. Data **12**, 387 (1967).

[2]T. S. Tolstova and T. V. Sheblom, Sb. Nauch. Tr., Gos. Inst. Prikl. Khim. (Leningrad) **20** (1975).

[3]I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976); Deposited Doc., VINITI 1951 (1976).

[4]M. J. Hampe, Chem.-Ing.-Tech. **57**, 669 (1985).

[5]R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**

J. W. Malone and R. W. Vining, J. Chem. Eng. Data **12**, 387–9 (1967).

**Variables:**

$T$/K = 298

**Prepared By:**

V. P. Sazonov

**Experimental Data**

The proportion of nitroethane in the water-rich phase at equilibrium at 298 K was reported to be 100 $w_1$ = 5.05. The corresponding mole fraction solubility, $x_1$, calculated by the compiler, is 0.0126. The proportion of nitroethane in the nitroethane-rich phase at equilibrium at 298 K was reported to be 100 $w_1$ = 99.14. The corresponding mole fraction solubility, $x_1$, calculated by the compiler, is 0.9651

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The titration method was used. No experimental details were reported.

**Source and Purity of Materials:**

(1) Commercial Solvents Corp.; purity 93.9 mass % with 2.3 mass % of 2-nitropropane.
(2) Distilled.

**Estimated Error:**

Temperature: ±1 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
T. S. Tolstova and T. V. Sheblom, Sb. Nauch. Tr., Gos. Inst. Prikl. Khim. (Leningrad) 20–3 (1975).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of nitroethane in water at 293 K was reported to be 100 $w_1$ = 4.5. The corresponding mole fraction, $x_1$, calculated by the compiler is 0.011.

The solubility of water in nitroethane at 293 K was reported to be 100 $w_2$ = 1.5. The corresponding mole fraction, $x_2$, calculated by the compiler is 0.059.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The titration method was used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purified by distillation over a column of 20 theoretical plates.
(2) Distilled.

**Estimated Error:**
Not reported.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976). *Deposited Doc., VINITI 1951 (1976).

**Variables:**
$T$/K = 295–444

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

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

| | | Water-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 22.0 | 295.2 | ··· | ··· | 99.2 | 0.967 |
| 30.0 | 303.2 | 4.5 | 0.011 | 98.9 | 0.956 |
| 41.0 | 314.2 | ··· | ··· | 98.6 | 0.944 |
| 50.0 | 323.2 | 5.5 | 0.014 | ··· | ··· |
| 55.0 | 328.2 | ··· | ··· | 98.0 | 0.922 |
| 62.0 | 335.2 | 6.4 | 0.016 | ··· | ··· |
| 64.0 | 337.2 | ··· | ··· | 97.8 | 0.914 |
| 71.0 | 344.2 | 7.0 | 0.018 | ··· | ··· |
| 80.0 | 353.2 | ··· | ··· | 96.0 | 0.852 |
| 135.0 | 408.2 | 20.0 | 0.057 | ··· | ··· |
| 150.0 | 423.2 | ··· | ··· | 80.7 | 0.501 |
| 159.0 | 432.2 | ··· | ··· | 77.0 | 0.446 |
| 160.0 | 433.2 | 35.0 | 0.114 | ··· | ··· |
| 164.0 | 437.2 | ··· | ··· | 70.0 | 0.359 |
| 167.5 | 440.7 | 45.0 | 0.164 | ··· | ··· |
| 168.0 | 441.2 | ··· | ··· | 67.5 | 0.333 |
| 169.0 | 442.2 | ··· | ··· | 60.0 | 0.263 |
| 169.5 | 442.7 | 50.0 | 0.194 | ··· | ··· |
| 170.5 | 443.7 | 55.0 | 0.227 | ··· | ··· |
| 170.5 | 443.7 | 55.0 | 0.227 | 55.0 | 0.227 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; distilled; $n$(20°C,D) = 1.3905, $d$(20°C,4°C) = 1.0525.
(2) Distilled; $n$(25°C,D) = 1.333.

**Estimated Error:**
Not reported.

**References:**
[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
M. J. Hampe, Chem.-Ing.-Tech. **57**, 669–81 (1985).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of nitroethane in water at 293 K was reported to be 100 $w_1$ = 4.68. The corresponding mole fraction, $x_1$ , calculated by the compiler is 0.0116.

The solubility of water in nitroethane at 293 K was reported to be 100 $w_2$ = 1.05. The corresponding mole fraction $x_2$ calculated by the compiler is 0.0424.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No details were reported.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.

**Estimated Error:**
Not reported.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
R. M. Stephenson, J. Chem. Eng. Data **37**, 80–95 (1992).

**Variables:**
$T$/K = 273–363

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Mutual solubility of nitroethane (1) and water (2)

| | | Water-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1$ | $x_1$ (compiler) | 100 $w_1$ | $x_1$ (compiler) |
| 0.0 | 273.2 | 4.32 | 0.0107 | 99.38 | 0.9747 |
| 9.2 | 282.4 | 4.22 | 0.0105 | 99.25 | 0.9695 |
| 19.6 | 292.8 | 4.38 | 0.0109 | 99.01 | 0.9600 |
| 31.0 | 304.2 | 4.44 | 0.0110 | 98.69 | 0.9476 |
| 40.6 | 313.8 | 4.60 | 0.0114 | 98.42 | 0.9373 |
| 50.5 | 323.7 | 5.19 | 0.0130 | 98.10 | 0.9253 |
| 60.8 | 334.0 | 5.40 | 0.0135 | 96.69 | 0.8752 |
| 70.4[a] | 343.6 | 5.82 | 0.0146 | 95.24 | 0.8277 |
| 80.4 | 353.6 | 6.27 | 0.0158 | 98.83 | 0.7850 |
| 90.1 | 363.3 | 6.55 | 0.0165 | 92.93 | 0.7593 |

[a]Below 70 °C the organic-rich is more dense than the water-rich phase; above 70 °C the water-rich phase is more dense.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No details were reported.

**Source and Purity of Materials:**
(1) Aldrich Chemical; not purified; purity 96 mass %.
(2) Twice distilled.

**Estimated Error:**
Temperature: to ±0.1 K;
Solubility: 0.01 mass % (1) in (2), 0.03 mass % (2) in (1).

## 3.2. 1,2-Ethanediol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$ ; [107-21-1]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

### Critical Evaluation

Solubilities in the system nitroethane (1) and 1,2-ethanediol (2) were reported in two publications. Francis[1] carried out measurement of the mutual solubilities of the two components between 273 and 341 K by the synthetic method. Zhuravlev and Erofeeva[2] studied the mutual solubilities of (1) and (2) between 299 and 342 K also by the synthetic method.

The upper critical solution temperature was reported as 341.2 K (Francis[1]) and 342.2 K (Zhuravlev and Erofeeva[2]). Thus, the recommended value is: $T_c$=(341.7±0.5) K. The corresponding critical solution composition was reported as $x_1$=0.483 (Francis[1]) and as $x_1$=0.517 (Zhuravlev and Erofeeva[2]).

All experimental values reported in Francis[1] and Zhuravlev and Erofeeva[2] (treated with the same weighing factor) have been approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1=1.18831,\ a_2=-1.07779,\ b_1=-4.94422,\ b_2=4.15935\ \text{(mean standard error of estimate was 0.0425)}.$$

For approximation $x_{c1}$ and UCST from Zhuravlev and Erofeeva[2] have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental points reported in Francis[1] and Zhuravlev and Erofeeva[2] are also presented in Fig. 2.

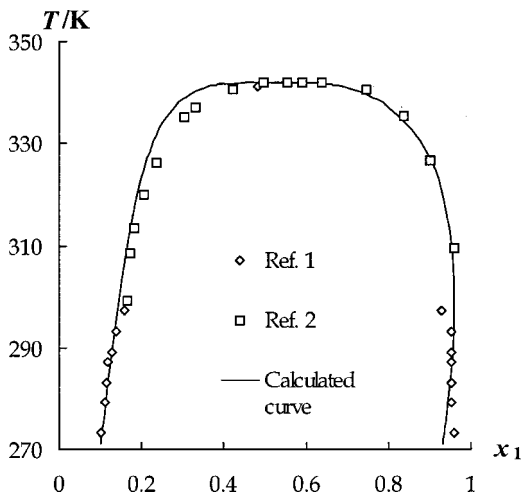


FIG. 2. Mutual solubility of nitroethane and 1,2-ethanediol.

Mutual solubility of nitroethane and 1,2-ethanediol

| | Glycol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|
| $T$/K | $x_1$ | 100 $w_1$ | $x_1$ | 100 $w_1$ |
| 273.2 | 0.104 | 12.3 | 0.691 | 73.0 |
| 283.2 | 0.119 | 14.0 | 0.735 | 77.0 |
| 293.2 | 0.135 | 15.9 | 0.764 | 79.7 |
| 303.2 | 0.152 | 17.8 | 0.786 | 81.6 |
| 313.2 | 0.172 | 20.1 | 0.856 | 87.8 |
| 323.2 | 0.199 | 23.1 | 0.896 | 91.2 |
| 328.2 | 0.218 | 25.2 | 0.921 | 93.4 |
| 333.2 | 0.244 | 28.1 | 0.949 | 95.7 |
| 338.2 | 0.291 | 33.2 | 0.959 | 96.6 |
| 339.2 | 0.306 | 34.8 | 0.958 | 96.5 |
| 340.2 | 0.327 | 37.0 | 0.950 | 95.8 |
| 341.2 | 0.360 | 40.5 | 0.936 | 94.6 |

**References:**

[1]A. W. Francis, J. Phys. Chem. **60**, 20 (1956).
[2]E. F. Zhuravlev and L. F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10 (1968).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

**Original Measurements:**
A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

**Variables:**
$T$/K = 273–341

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1,2-ethanediol (2)

| | | Glycol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 0.0 | 273.2 | 12.0 | 0.101 | 96.5 | 0.958 |
| 6.0 | 279.2 | 13.0 | 0.110 | 96.0 | 0.952 |
| 10.0 | 283.2 | 13.5 | 0.114 | 96.0 | 0.952 |
| 14.0 | 287.2 | 14.0 | 0.119 | 96.0 | 0.952 |
| 16.0 | 289.2 | 15.0 | 0.127 | 96.0 | 0.952 |
| 20.0 | 293.2 | 16.5 | 0.140 | 96.0 | 0.952 |
| 24.0 | 297.2 | 18.5 | 0.158 | 94.0 | 0.928 |
| 68.0 | 341.2 | 53.0 | 0.483 | 53.0 | 0.483 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Observations were made after vigorous shaking in glass stoppered 15 mL graduated tubes, immersed in water baths in large Dewar flasks. Water was agitated with a rapid stream of air bubbles. Temperature was adjusted by adding cooler or warmer water occasionally.

**Source and Purity of Materials:**
(1) Eastman Kodak Co.; distilled with 30 cm column with reflux; boiling point=114–115 °C, $n$(20 °C,D)=1.3920, $\rho$(20 °C)=1046.9 g·L$^{-1}$.
(2) Source not specified; purified by crystallization; melting point=−13.3 °C, $n$(20 °C,D)=1.4315, $\rho$(20 °C)=1110.1 g·L$^{-1}$.

**Estimated Error:**
Not specified.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

**Original Measurements:**
E. F. Zhuravlev and L. F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10–7 (1968).

**Variables:**
$T$/K = 299–342

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1,2-ethanediol (2)

| | | Glycol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 26.0 | 299.2 | 19.2 | 0.164 | ··· | ··· |
| 35.2 | 308.4 | 20.0 | 0.171 | ··· | ··· |
| 36.5 | 309.7 | ··· | ··· | 96.7 | 0.960 |
| 40.1 | 313.3 | 21.4 | 0.184 | ··· | ··· |
| 46.9 | 320.1 | 23.9 | 0.206 | ··· | ··· |
| 53.0 | 326.2 | 27.1 | 0.235 | ··· | ··· |
| 53.6 | 326.8 | ··· | ··· | 91.8 | 0.903 |
| 62.0 | 335.2 | 34.5 | 0.303 | ··· | ··· |
| 62.2 | 335.4 | ··· | ··· | 86.2 | 0.838 |
| 64.1 | 337.3 | 37.4 | 0.331 | ··· | ··· |
| 67.5 | 340.7 | 47.0 | 0.423 | 77.9 | 0.745 |
| 68.8 | 342.0 | ··· | ··· | 68.0 | 0.637 |
| 68.9 | 342.1 | ··· | ··· | 63.5 | 0.590 |
| 69.0 | 342.2 | 54.3 | 0.495 | 60.1 | 0.555 |
| 69.0 | 342.2 | 56.4 | 0.517 | 56.4 | 0.517 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; distilled.
(2) Source not specified; distilled.

**Estimated Error:**
Not specified.

## 3.3. 1,2,3-Propanetriol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2,3-Propanetriol; $C_3H_8O_3$; [56-81-51]

**Original Measurements:**
L. F. Erofeeva and E. F. Zhuravlev, Uch. Zap., Perm. Gos. Univ. **178**, 18–22 (1968).

**Variables:**
$T$/K = 299–383

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1,2,3-propanetriol (2)

| | | Glycerol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 26.0 | 299.2 | 2.9 | 0.035 | ··· | ··· |
| 29.0 | 302.2 | 3.2 | 0.039 | ··· | ··· |
| 44.0 | 317.2 | 4.2 | 0.051 | ··· | ··· |
| 73.0 | 346.2 | 6.5 | 0.079 | ··· | ··· |
| 83.0 | 356.2 | ··· | ··· | 99.0 | 0.092 |
| 103.0 | 376.2 | 10.0 | 0.120 | ··· | ··· |
| 110.0 | 383.2 | ··· | ··· | 98.5 | 0.988 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; distilled.
(2) Source not specified; distilled.

**Estimated Error:**
Not specified.

## 3.4. 2,2′-Iminobisethanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 2,2′-Iminobisethanol; $C_4H_{11}NO_2$; [111-42-2]

**Original Measurements:**
L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 7–11 (1971).

**Variables:**
$T$/K = 298–363

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**
Mutual solubility of nitroethane (1) and 2,2′-iminobisethanol (2)

| | | Iminobisethanol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 24.9 | 298.1 | 21.3 | 0.275 | ··· | ··· |
| 34.4 | 306.6 | ··· | ··· | 96.9 | 0.978 |
| 51.6 | 324.8 | 25.6 | 0.325 | ··· | ··· |
| 63.8 | 337.0 | ··· | ··· | 95.0 | 0.964 |
| 68.9 | 342.1 | 33.5 | 0.414 | ··· | ··· |
| 76.9 | 350.1 | ··· | ··· | 91.5 | 0.938 |
| 79.4 | 352.6 | 41.6 | 0.499 | ··· | ··· |
| 83.1 | 356.3 | ··· | ··· | 86.9 | 0.903 |
| 85.6 | 358.8 | 49.4 | 0.578 | ··· | ··· |
| 86.9 | 360.1 | 51.9 | 0.602 | 82.2 | 0.866 |
| 89.4 | 362.6 | ··· | ··· | 72.5 | 0.787 |
| 89.7 | 362.9 | 60.6 | 0.683 | ··· | ··· |
| 90.0 | 363.2 | 68.0 | 0.749 | 68.0 | 0.749 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; distilled.
(2) Source not specified; distilled.

**Estimated Error:**
Not specified.

## 3.5. Cyclohexane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Cyclohexane; $C_6H_{12}$ ; [110-82-7]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Solubilities in the system nitroethane+cyclohexane were reported in the three publications listed in Table 1.

Table 1. Summary of solubility data for the system nitroethane+cyclohexane

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Erofeeva and Yunnikova[1] | 276–296 | mutual | synthetic |
| Clever *et al.*[2] | 279–298 | mutual | synthetic |
| Kawate and Nakata[3] | 290–296 | mutual | synthetic |

All original data are compiled in the data sheets immediately following this Critical Evaluation. All reported data are included in Tables 2 and 3. Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). "Best" values are arithmetic means. The uncertainty limits ($\sigma_n$) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits. The letter (R) designates "recommended" data. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Tentative and recommended (R) values for the solubility nitroethane (1) in cyclohexane (2)

| $T$/K | Solubility, 100 $w_1$ Reported values | "Best" values ($\pm\sigma_n$) 100 $w_1$ | $x_1$ |
|---|---|---|---|
| 278.2 | 7.6* (Ref. 1) | 7.6 | 0.084 |
| 283.2 | 11.0 (Ref. 1) | 11.0 | 0.122 |
| 288.2 | 14.9* (Ref. 1) | 14.9 | 0.164 |
| 290.2 | 17.7* (Ref. 1), 16.9* (Ref. 3) | 17.3±0.4 (R) | 0.190 |
| 292.2 | 21.6* (Ref. 1), 19.8* (Ref. 3) | 20.7±0.7 (R) | 0.226 |
| 293.2 | 24.0* (Ref. 1), 21.2* (Ref. 3) | 22.6±1.4 | 0.247 |
| 294.2 | 28.5* (Ref. 1), 24.1* (Ref. 3) | 26±2 | 0.283 |
| 295.2 | 37.1* (Ref. 1), 28.1* (Ref. 3) | 33±4 | 0.356 |

Table 3. Tentative and recommended (R) values for the solubility cyclohexane (2) in nitroethane (1)

| $T$/K | Solubility, 100 $w_2$ Reported values | "Best" values ($\pm\sigma_n$) 100 $w_2$ | $x_2$ |
|---|---|---|---|
| 278.2 | 18.2* (Ref. 1), 19.8* (Ref. 2) | 19.0±0.8 (R) | 0.173 |
| 283.2 | 22.7* (Ref. 1), 24.1* (Ref. 2) | 23.4±0.7 (R) | 0.214 |
| 288.2 | 28.0* (Ref. 1), 28.8* (Ref. 2) | 28.4±0.4 (R) | 0.261 |
| 290.2 | 30.4* (Ref. 1), 30.2* (Ref. 2), 30.8* (Ref. 3) | 30.5±0.3 (R) | 0.281 |
| 292.2 | 32.8* (Ref. 1), 32.2* (Ref. 2), 34.5 (Ref. 3) | 33.2±1 (R) | 0.307 |
| 293.2 | 35.1* (Ref. 1), 33.9* (Ref. 2), 36.5* (Ref. 3) | 35.2±1 (R) | 0.326 |
| 294.2 | 38.0* (Ref. 1), 36.0* (Ref. 2), 40.0* (Ref. 3) | 38±2 | 0.354 |
| 295.2 | 43.6*(Ref. 1), 39.2* (Ref. 2), 43.4 (Ref. 3) | 42±2 (R) | 0.392 |

The interpolated values reported in the tables above were approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1=0.95104,\ a_2=-0.53288,\ b_1=-0.17250,\ b_2=-0.00943\ \text{(mean standard error of estimate was 0.0098)}.$$

For this approximation the recommended values of UCST and $x_{c1}$ have been used. The calculated relationship is presented in Fig. 3 together with the "best" values from the above tables.

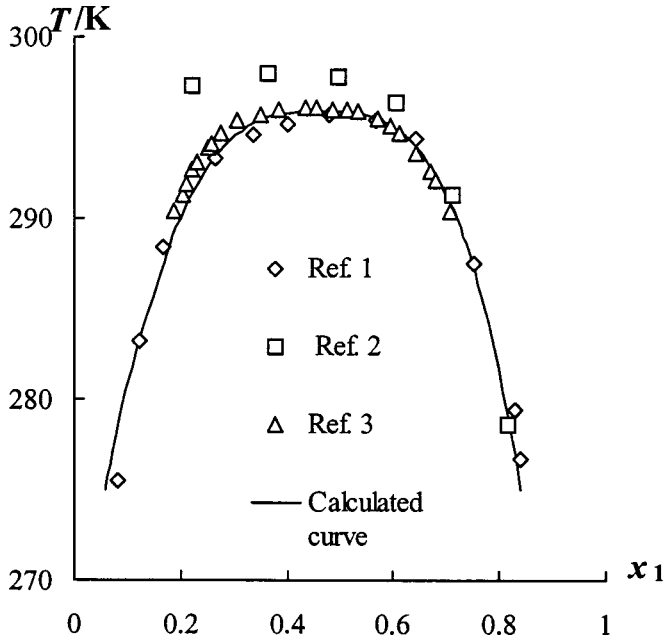


FIG. 3. Mutual solubility of nitroethane and cyclohexane.

The upper critical solution temperature has been reported as 295.7 K,[1] 296.05 K,[3] and 298.2 K,[2] The UCST of Clever *et al.*[2] is rejected. Thus, the recommended values are: $T_c$=295.9±0.2 K.

The corresponding critical solution composition has been reported as $x_{c1}$=0.448 (Kawate and Nakata[3]) and $x_{c1}$=0.478.[1] The data average $x_{c1}$=0.463±0.015. This value is recommended.

**References:**

[1]L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 7 (1971).
[2]H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31 (1972).
[3]K. Kawate and M. Nakata, J. Phys. Chem. **166**, 195 (1990).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Cyclohexane; $C_6H_{12}$ ; [110-82-7]

**Original Measurements:**
L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 7–11 (1971).

**Variables:**
$T$/K = 276–296

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**
Mutual solubility of nitroethane (1) and cyclohexane (2)

| | | Cyclohexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 2.3 | 275.5 | 7.5 | 0.083 | ··· | ··· |
| 3.5 | 276.7 | ··· | ··· | 82.5 | 0.841 |
| 6.2 | 279.4 | ··· | ··· | 81.2 | 0.829 |
| 10.0 | 283.2 | 11.0 | 0.122 | ··· | ··· |
| 14.3 | 287.5 | ··· | ··· | 72.8 | 0.750 |
| 15.2 | 288.4 | 15.0 | 0.165 | ··· | ··· |
| 20.1 | 293.3 | 24.3 | 0.265 | ··· | ··· |
| 21.2 | 294.4 | ··· | ··· | 61.5 | 0.642 |
| 21.4 | 294.6 | 31.2 | 0.337 | ··· | ··· |
| 22.0 | 295.2 | 37.3 | 0.400 | ··· | ··· |
| 22.2 | 295.4 | ··· | ··· | 53.9 | 0.567 |
| 22.5 | 295.7 | 45.0 | 0.478 | 45.0 | 0.478 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; distilled.
(2) Source not specified; distilled.

**Estimated Error:**
Not specified.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Cyclohexane; $C_6H_{12}$ ; [110-82-7]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 279–298

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and cyclohexane (2)

| | | Cyclohexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ (compilers) | $x_1$ | 100 $w_1$ (compilers) | $x_1$ |
| 5.4 | 278.6 | ··· | ··· | 79.7 | 0.815 |
| 18.1 | 291.3 | ··· | ··· | 68.6 | 0.710 |
| 23.2 | 296.4 | ··· | ··· | 57.7 | 0.605 |
| 24.1 | 297.3 | 20.1 | 0.220 | ··· | ··· |
| 24.6 | 297.8 | ··· | ··· | 46.6 | 0.495 |
| 24.8 | 298.0 | ··· | ··· | 33.9 | 0.365 |
| 25.0 | 298.2 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solutions of (1) and (2) were prepared by weight from glass syringes in 13 mm×100 mm Kimax screw cap culture tubes and sealed by a cap with a Teflon faced rubber liner. The tubes were suspended in a 3 L well-stirred water bath and cloud points observed visually. At least two observations were made of each set of samples, the first at a relatively fast cooling rate to find the approximate cloud point temperature and the second at a slow cooling rate to more precisely determine the cloud point temperature.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled at 57 °C/12.9 kPa.
(2) Fisher; dried over $CaSO_4$ and distilled at atmospheric pressure from $CaH_2$ .

**Estimated Error:**
Temperature: ±0.1 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Cyclohexane; $C_6H_{12}$ ; [110-82-7]

**Original Measurements:**
K. Kawate and M. Nakata, J. Phys. Chem. **166**, 195–209 (1990).

**Variables:**
$T$/K= 290–296

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The mutual solubility of nitroethane (1) and cyclohexane (2) in volume fractions is presented over the temperature range in graphical form. This table is based on numerical data provided by Dr. M. Nakata at the request of the compiler.

Mutual solubility of nitroethane (1) and cyclohexane (2)

| | | Cyclohexane-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | $\varnothing_1$ | $x_1$ (compiler) | 100 $w_1$ (compiler) | $\varnothing_1$ | $x_1$ (compiler) | 100 $w_1$ (compiler) |
| 17.20 | 290.35 | 0.131 | 0.186 | 16.9 | ··· | ··· | ··· |
| 17.28 | 290.43 | ··· | ··· | ··· | 0.616 | 0.708 | 68.4 |
| 18.19 | 291.34 | 0.144 | 0.204 | 18.6 | ··· | ··· | ··· |
| 18.80 | 291.95 | 0.149 | 0.210 | 19.2 | ··· | ··· | ··· |
| 18.99 | 292.14 | ··· | ··· | ··· | 0.584 | 0.680 | 65.5 |
| 19.42 | 292.57 | ··· | ··· | ··· | 0.572 | 0.670 | 64.4 |
| 19.57 | 292.72 | 0.159 | 0.222 | 20.3 | ··· | ··· | ··· |
| 20.00 | 293.15 | 0.166 | 0.232 | 21.2 | ··· | ··· | ··· |
| 20.48 | 293.63 | ··· | ··· | ··· | 0.544 | 0.644 | 61.7 |
| 20.73 | 293.88 | 0.182 | 0.253 | 23.2 | ··· | ··· | ··· |
| 20.97 | 294.12 | 0.186 | 0.257 | 23.6 | ··· | ··· | ··· |
| 21.51 | 294.66 | ··· | ··· | ··· | 0.509 | 0.612 | 58.4 |
| 21.57 | 294.72 | 0.201 | 0.276 | 25.4 | ··· | ··· | ··· |
| 21.96 | 295.11 | ··· | ··· | ··· | 0.491 | 0.594 | 56.6 |
| 22.20 | 295.35 | 0.225 | 0.306 | 28.2 | ··· | ··· | ··· |
| 22.31 | 295.46 | ··· | ··· | ··· | 0.468 | 0.572 | 54.4 |
| 22.51 | 295.66 | 0.262 | 0.351 | 32.5 | ··· | ··· | ··· |
| 22.70 | 295.85 | ··· | ··· | ··· | 0.430 | 0.534 | 50.5 |
| 22.81 | 295.96 | ··· | ··· | ··· | 0.409 | 0.513 | 48.4 |
| 22.83 | 295.98 | 0.292 | 0.385 | 35.8 | ··· | ··· | ··· |
| 22.89 | 296.04 | ··· | ··· | ··· | 0.383 | 0.485 | 45.6 |
| 22.90 | 296.05 | 0.338 | 0.437 | 40.9 | ··· | ··· | ··· |
| 22.90 | 296.05 | ··· | ··· | ··· | 0.356 | 0.456 | 42.8 |

The upper critical solution temperature was reported to be 22.9 °C at $\varnothing_1 = 0.35$ (100 $w_1 = 42.0$ and $x_1 = 0.448$: compiler).

For conversions of volume concentration utilized values of density of nitroethane $\rho$(20 °C)=1052.8 g·L$^{-1}$ from Weissberger *et al.*[1] and cyclohexane $\rho$(20 °C)=778.4 g·L$^{-1}$ from Timmermans[2] at 293.2 K (20.0 °C).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. A number of glass tubes containing known weight mixtures were prepared to determine a coexistence curve. To minimize scattering of data due to traces of impurities, a new cell was devised for the visual method. It has a main tube of 0.5 cm inside diameter and 20 cm length and a side tube of 12 cm length and of the same volume as the main one. The cell was dried, 3 mL of (2) introduced into the side tube, and 0.4 mL of (1) into the main tube. The cell was sealed with a greased tapered joint. The volume of (1) in the main tube was determined from the meniscus height (error ±0.3%). Then, the (2) in the side tube was transferred step by step into the main tube by inclining the cell. At each step, composition was determined from meniscus height. The cell was in a water bath to determine phase separation temperature.

**Source and Purity of Materials:**
(1) Source not specified; dried over calcium chloride and fractionally distilled at reduced pressure under nitrogen gas; no impurity detectable by gas chromatography.
(2) Source not specified; passed through silica gel and fractionally distilled in a 1.8 cm×100 cm column packed with Rashig rings.

**Estimated Error:**
Temperature: control to ±0.01 K.

**References:**
[1]A. Weissberger, E. S. Proskauer, J. A. Riddick, and E. E. Toops, Jr., *Organic Solvents* (Interscience, New York, 1955).
[2]J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

## 3.6. 1-Hexene

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Hexene; $C_6H_{12}$ ; [592-41-6]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 230–245

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-hexene (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| −43.0 | 230.2 | 11.7 | 0.129 | 78.8 | 0.806 |
| −38.4 | 234.8 | 14.3 | 0.158 | 73.6 | 0.758 |
| −34.0 | 239.2 | 17.8 | 0.195 | 68.3 | 0.707 |
| −30.0 | 243.2 | 25.4 | 0.276 | 59.0 | 0.617 |
| −29.9[a] | 243.3 | 27.05 | 0.294 | ··· | ··· |
| −29.8[a] | 243.4 | ··· | ··· | 59.19 | 0.619 |
| −29.0[a] | 244.2 | ··· | ··· | 53.50 | 0.563 |
| −28.6[a] | 244.8 | 35.89 | 0.386 | ··· | ··· |
| −28.5[a] | 244.7 | 43.98 | 0.468 | ··· | ··· |
| −28.5 | 244.7 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corporation; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Philips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to ±0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**
[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

## 3.7. 2-Methylpentane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2-Methylpentane; $C_6H_{14}$ ; [107-83-5]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 273–300

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 2-methylpentane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| −0.35 | 272.80 | ··· | ··· | 86.3 | 0.879 |
| 2.05 | 275.20 | 8.4 | 0.095 | ··· | ··· |
| 3.80 | 276.95 | ··· | ··· | 84.9 | 0.866 |
| 6.30 | 279.45 | 10.1 | 0.114 | ··· | ··· |
| 8.00 | 281.15 | ··· | ··· | 83.1 | 0.850 |
| 8.75 | 281.90 | 11.0 | 0.124 | ··· | ··· |
| 10.85 | 284.00 | ··· | ··· | 81.4 | 0.834 |
| 11.20 | 284.35 | 12.3 | 0.139 | ··· | ··· |
| 13.70 | 286.85 | ··· | ··· | 79.9 | 0.820 |
| 13.75 | 286.90 | 14.3 | 0.161 | ··· | ··· |
| 15.95 | 289.10 | 15.7 | 0.176 | ··· | ··· |
| 17.80 | 289.95 | ··· | ··· | 76.4 | 0.788 |
| 19.00 | 292.15 | 18.8 | 0.210 | ··· | ··· |
| 20.00 | 293.15 | ··· | ··· | 74.1 | 0.767 |
| 20.25 | 293.40 | 20.8 | 0.232 | ··· | ··· |
| 21.00 | 294.15 | 21.8 | 0.242 | ··· | ··· |
| 23.4[a] | 296.55 | ··· | ··· | 69.28 | 0.721 |
| 24.00 | 297.15 | ··· | ··· | 67.6 | 0.705 |
| 24.20 | 297.35 | 28.4 | 0.313 | ··· | ··· |
| 25.20 | 298.35 | ··· | ··· | 63.8 | 0.669 |
| 25.3[a] | 298.45 | 30.31 | 0.333 | ··· | ··· |
| 25.50 | 298.65 | 32.0 | 0.351 | ··· | ··· |
| 25.6[a] | 298.75 | 31.81 | 0.349 | ··· | ··· |
| 25.8[a] | 298.95 | ··· | ··· | 61.88 | 0.651 |
| 26.2[a] | 299.35 | 34.06 | 0.372 | ··· | ··· |
| 26.6[a] | 299.75 | 37.07 | 0.403 | ··· | ··· |
| 26.6[a] | 299.75 | 42.17 | 0.456 | ··· | ··· |
| 26.7[a] | 299.85 | 46.69 | 0.501 | 57.59 | 0.609 |
| 26.7[a] | 299.85 | ··· | ··· | 53.12 | 0.565 |
| 26.7[a] | 299.85 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**

(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Philips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**

Temperature: to ±0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**

[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

## 3.8. 3-Methylpentane

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$; [96-14-0]

**Evaluator:**

V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system nitroethane+3-methylpentane were reported in the publications listed in Table 1.

Table 1. Summary of solubility data for the system nitroethane+3-methylpentane

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Wims *et al.*[1] | 297–300 | mutual | synthetic |
| Stein *et al.*[2] | 299.574 | USCT | synthetic |
| Tsai and McIntyre[3] | 299.692 | UCST | synthetic |
| Reeder *et al.*[4] | 298.596 | mutual | not stated |
| Balasubramanaian and Mitra[5] | 293.2 | UCST | titration |
| Beysens and Tufeu[6] | 300–301 | UCST | synthetic |
| Khosla and Widom[7] | 299.600 | UCST | synthetic |
| Burstyn and Sengers[8] | 299.545 | UCST | synthetic |
| Tanaka and Wada[9] | 299.09 | UCST | synthetic |

Reeder *et al.*[4] studied of the excess volumes of mixtures of (1) and (2) at 298.596 K. Beysens and Tufeu[6] determined of the variation of the critical temperature as a function of pressure (from 500 to 12 500 kPa). Khosla and Widom[7] determined the densities and surface tensions of the equilibrium liquid phases critical mixture of (1) and (2) between 288 and 300 K. Pegg and McLure[10] studied shear viscosities and densities of the equilibrium liquid phases in critical mixtures of (1) and (2) between 292 and 300 K. Apart from one further publication[8] which did not contain sufficient information to justify inclusion, all original data are compiled in the data sheets immediately following this Critical Evaluation.

All experimental values reported in Wims *et al.*[1] (treated with the same weighing factor) were approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived: $a_1=0.969\,85$, $a_2=-0.596\,64$, $b_1=-0.000\,33$, $b_2=-0.734\,08$ (mean standard error of estimate was 0.0051).

For this approximation $x_{c1}$ and UCST from five references[1–3,6,8] were used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for selected temperatures are presented in Table 2. This relationship together with experimental points reported in Wims *et al.*[1] is also presented in Fig. 4.

Table 2. Mutual solubility of nitroethane and 3-methylpentane

| | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|
| $T$/K | $x_1$ | $100\,w_1$ | $x_1$ | $100\,w_1$ |
| 297.0 | 0.287 | 26.0 | 0.692 | 66.2 |
| 297.5 | 0.302 | 27.4 | 0.680 | 64.9 |
| 298.0 | 0.320 | 29.1 | 0.666 | 63.5 |
| 298.5 | 0.342 | 31.2 | 0.648 | 61.6 |
| 299.0 | 0.372 | 34.0 | 0.622 | 58.9 |
| 299.1 | 0.380 | 34.8 | 0.615 | 58.2 |
| 299.2 | 0.388 | 35.7 | 0.608 | 57.5 |
| 299.3 | 0.399 | 36.6 | 0.598 | 56.4 |
| 299.4 | 0.412 | 37.9 | 0.586 | 55.2 |
| 299.5 | 0.430 | 39.6 | 0.569 | 53.5 |

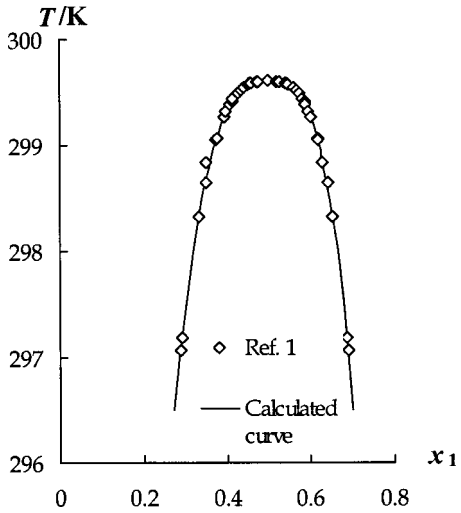


FIG. 4. Mutual solubility of nitroethane and 3-methylpentane.

The upper critical solution temperature has been reported as 293.2 K (Balasubramanaian and Mitra[5]), 299.09 K (Burstyn and Sengers[8]), 299.545 K,[7] 299.574 K,[2] 299.600 K,[6,9] 299.608 and 299.622 K [Wims *et al.*,[1] two methods] and 299.692 K.[3] The data of Balasubramanaian and Mitra[5] are in marked disagreement with all other studies and are rejected. The UCST of Tanaka and Wada,[8] also is rejected. Thus, the recommended value are: $T_c = 299.604 \pm 0.032$ K.

The corresponding critical solution composition has been reported as $x_{c1} = 0.500$.[1–3,6,8] This value is recommended.

**References:**

[1]A. M. Wims, D. McIntyre, and F. Hynne, J. Chem. Phys. **50**, 616 (1969).
[2]A. Stein, J. C. Allegra, and G. F. Allen, Chem. Phys. **55**, 4265 (1971).
[3]B. C. Tsai and D. J. McIntyre, Chem. Phys. **60**, 937 (1974).
[4]J. Reeder, T. E. Block, and C. M. Knobler, J. Chem. Thermodyn. **8**, 133 (1976).
[5]D. Balasubramanaian and P. Mitra, J. Phys. Chem. **83**, 2724 (1979).
[6]D. Beysens and R. Tufeu, Rev. Phys. Appl. **14**, 907 (1979).
[7]M. P. Khosla and B. Widom, J. Colloid Interface Sci. **76**, 375 (1980).
[8]H. C. Burstyn and J. V. Sengers, Phys. Rev. A. Gen. Phys. **55**, 448 (1982).
[9]H. Tanaka and Y. Wada, Chem. Phys. **78**, 143 (1983).
[10]I. J. Pegg and I. A. McLure, Mol. Phys. **53**, 897 (1984).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$; [96-14-0]

**Original Measurements:**
A. M. Wims, D. McIntyre, and F. Hynne, J. Chem. Phys. **50**, 616–20 (1969).

**Variables:**
$T$/K = 297–300

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Mutual solubility and densities of the equilibrium liquid phases of system nitroethane (1) + 3-methylpentane (2)

| | | Hydrocarbon-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | 100 $w_1$ (compilers) | $\rho$(g·L$^{-1}$) | $x_1$ | 100 $w_1$ (compilers) | $\rho$(g·L$^{-1}$) |
| 23.905 | 297.055 | 0.289 | 26.1 | 730.5 | 0.692 | 66.7 | 871.0 |
| 24.032 | 297.182 | 0.292 | 26.4 | 731.2 | 0.687 | 65.7 | 868.6 |
| 25.176 | 298.326 | 0.333 | 30.3 | 741.6 | 0.654 | 62.2 | 853.2 |
| 25.495 | 298.645 | 0.349 | 31.8 | 746.0 | 0.642 | 61.0 | 847.7 |
| 25.678 | 298.828 | 0.350 | 32.8 | 748.8 | 0.631 | 59.8 | 843.2 |
| 25.901 | 299.051 | 0.375 | 34.3 | 753.2 | 0.618 | 58.5 | 837.4 |
| 25.914 | 299.064 | 0.377 | 34.5 | 753.8 | 0.619 | 58.6 | 837.9 |
| 26.108 | 299.258 | 0.394 | 36.2 | 758.9 | 0.604 | 57.1 | 832.0 |
| 26.161 | 299.311 | 0.399 | 36.6 | 760.3 | 0.597 | 56.3 | 829.1 |
| 26.229 | 299.379 | 0.408 | 37.5 | 763.2 | 0.588 | 55.4 | 825.5 |
| 26.262 | 299.412 | 0.415 | 38.2 | 765.2 | 0.589 | 55.5 | 825.8 |
| 26.281 | 299.431 | 0.417 | 38.4 | 765.7 | 0.581 | 54.7 | 822.6 |
| 26.340 | 299.490 | 0.430 | 39.7 | 769.8 | 0.576 | 54.2 | 820.9 |
| 26.364 | 299.514 | 0.436 | 40.2 | 771.7 | 0.567 | 53.3 | 817.3 |
| 26.389 | 299.539 | 0.441 | 40.7 | 773.3 | 0.562 | 52.8 | 815.5 |
| 26.422 | 299.572 | 0.452 | 41.8 | 777.1 | 0.549 | 51.5 | 810.5 |
| 26.428 | 299.578 | 0.455 | 42.1 | 777.9 | 0.544 | 51.0 | 809.0 |
| 26.439 | 299.589 | 0.460 | 42.6 | 779.6 | 0.540 | 50.6 | 807.5 |
| 26.449 | 299.599 | 0.473 | 43.9 | 784.0 | 0.527 | 49.3 | 802.5 |
| 26.454 | 299.604 | 0.476 | 44.2 | 784.8 | 0.522 | 48.8 | 800.8 |
| 26.458 | 299.608 | 0.500 | 46.6 | ··· | 0.500 | 46.6 | ··· (UCST) |
| 26.472[a] | 299.622 | ··· | ··· | ··· | ··· | ··· | ··· (UCST) |

[a]From visual determination. Data from visual determinations are in a graphical form.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The visual and float techniques were used to determine the coexistence curve. Mixtures of different compositions were made up in glass cells under a nitrogen atmosphere. Separation temperature was determined for each cell in a 100 gallon (379 L) bath. A more precise determination of the coexistence curve was made by using a magnetically suspended float technique. Density measurements were made in the cylindrical portion of the cell with a sealed glass float containing a ferromagnetic slug of metal.

**Source and Purity of Materials:**
(1) Source not specified; distilled on a packed, or a spinning-band column at reduced pressures; no impurities by gas chromatography.
(2) Source not specified; research-grade; purity 99.9 mass %; not purified.

**Estimated Error:**
Temperature: ±0.001 K,
Density: ±0.1 g·L$^{-1}$.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
A. Stein, J. C. Allegra, and G. F. Allen, J. Chem. Phys. **55**, 4265–9 (1971).

**Variables:**
$T$/K = 299.574

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The upper critical solution temperature was reported to be 26.424 °C (299.692 K, compilers) at $x_1 = 0.5000$ (100 $w_1 = 46.56$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The critical separation temperatures were determined by visual observation of the appearance of a meniscus. Critical temperatures determined in separate closed tubes and in the viscometers agreed within experimental error. Solutions were prepared from weighed amounts of the pure components. All manipulations were carried out in a dry box to eliminate contamination by moisture.

**Source and Purity of Materials:**
(1) Purified by double distillation and by preparative gas chromatography; purity 99.97 mole % by GLC.
(2) Phillips; research grade; purity 99.99 mole %.

**Estimated Error:**
Temperature: control to ±0.001 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
B. C. Tsai and D. McIntyre, J. Chem. Phys. **60**, 937–45 (1974).

**Variables:**
$T$/K = 299.692

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The upper critical solution temperature was reported to be 26.542 °C (299.692 K, compilers) at $x_1 = 0.5000$ (100 $w_1 = 46.56$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The phase separation temperature for a critical composition was determined both in a separate cell and in a viscosimeter. Both critical temperatures were equal.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell Co.; 0.01 mass % impurities detectable by GLC.
(2) Phillips; research grade; purity 99.99 mole % by GLC.

**Estimated Error:**
Temperature: control to ±0.001 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
J. Reeder, T. E. Block, and C. M. Knobler, J. Chem. Thermodyn. **8**, 133–40 (1976).

**Variables:**
$T$/K = 298.596

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The solubility of nitroethane in 3-methylpentane at 298.596 K was reported to be $x_1 = 0.3627$. The corresponding mass percentage calculated by the compilers is 100 $w_1 = 33.14$.

The solubility of nitroethane in 3-methylpentane at 298.596 K was reported to be $x_2 = 0.2958$. The corresponding mass percentage calculated by the compilers is 100 $w_2 = 32.53$.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
These data are from a study of the excess volumes of (1) and (2) mixtures. A detailed study of the apparatus and procedure is in Reeder *et al.*[1]

**Source and Purity of Materials:**
(1) Obtained from Dr. S. Greer of the US National Bureau of Standards; 99.95 mole % purity; dried and degassed by vacuum sublimation.
(2) Phillips Petroleum Co.; research grade; 99.99 mole % purity; not purified.

**Estimated Error:**
Not specified.

**References:**
[1]J. Reeder, C. M. Knobler, and R. L. Scott, J. Chem. Thermodyn. **7**, 345 (1975).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
D. Beysens and R. Tufeu, Rev. Phys. Appl. **14**, 907–9 (1979).

**Variables:**
$T$/K = 300–301; $P$/kPa = 500–12500

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The variation of the critical temperature as a function of pressure in the critical mixture (1) and (2) over the temperature and pressure range were presented in a graphical form in original publication. The numerical data in the table below were extracted graphically by the compiler.

Effect of pressure on the solubility of mixture nitroethane (1) and 3-methylpentane (2)

| 100 $w_1$ | $x_1$ (compiler) | $P$/kPa | $T$/K | $t$/°C(compiler) |
|---|---|---|---|---|
| 46.9 | 0.503 | 500 | 300.27 | 27.12 |
| | | 2500 | 300.32 | 27.17 |
| | | 5000 | 300.45 | 27.30 |
| | | 7500 | 300.49 | 27.34 |
| | | 10 000 | 300.61 | 27.46 |
| | | 12 500 | 300.68 | 27.53 |

A value of $dT_c dP$ of $3.7 \pm 0.5\ 10^{-8}$ K·Pa$^{-1}$ was reported in the above pressure range.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The mixture was mixed by heating the glass tube and varying the pressure; then the thermostat was set at a temperature high enough so that the mixture remained in the one phase region when the desired pressure was applied. When the thermal equilibrium was reached, the temperature was lowered. Another equilibrium takes place and an observation was done in order to detect the meniscus. If it is not visible, another step was performed.

**Source and Purity of Materials:**
(1) Source not specified; purity 96.0 mass %; distilled; the impurity level less than 0.5 mass % by chromatography and NMR.
(2) Source not specified; reagent for gas chromatography; not purified.

**Estimated Error:**
Temperature: ±0.01 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
D. Balasubramanaian and P. Mitra, J. Phys. Chem. **83**, 2724–7 (1979).

**Variables:**
$T$/K = 293

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The upper critical solution temperature was reported to be 20 °C (293 K) at $x_1 = 0.500$ (100 $w_1 = 46.6$ compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Probably the titration method was used. The details of the measurements described in Hales *et al.*[1]

**Source and Purity of Materials:**
(1) Source not specified; best analytical grade.
(2) Source not specified; best analytical grade.

**Estimated Error:**
Not specified.

**References:**
[1]B. J. Hales, G. L. Bertrand, and L. G. Hepler, J. Phys. Chem. **70**, 3970 (1966).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
M. P. Khosla and B. Widom, J. Colloid Interface Sci. **76**, 75–92 (1980).

**Variables:**
$T$/K = 288–299

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Densities and surface tensions of the equilibrium liquid phases system nitroethane (1) +3-methylpentane (2)

| $t$/°C | $T$/K (compilers) | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| | | $\rho$(g·L$^{-1}$) | $\sigma$ (dyn/cm) | $\rho$(g·L$^{-1}$) | $\sigma$ (dyn/cm) |
| 15.089 | 288.239 | 708.1 | 19.16 | 930.8 | 19.73 |
| 20.005 | 293.155 | 716.3 | 18.66 | 903.3 | 19.00 |
| 22.006 | 295.156 | 723.7 | 18.56 | 887.4 | 18.70 |
| 25.004 | 298.154 | ··· | 18.21 | ··· | 18.33 |
| 26.005 | 299.155 | 753.4 | 18.12 | 836.4 | 18.19 |
| 26.203 | 299.353 | ··· | 18.14 | ··· | 18.14 |

UCST is 26.450 °C at $x_1 = 0.500$ (100 $w_1 = 46.6$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Mixtures of near-critical composition were made in glass tubes, closed at one end and joined to vacuum-tight Teflon-glass valves. Phase-separation temperatures were determined visually. The critical composition sample was the one most opalescent at its phase-separation temperature. Two different pycnometers, volumes 25 and 50 mL, of the type glass-bulb-to-capillary, were used to determine densities of mixtures. Surface tension was measured by the differential-capillary-rise method using a sample cell adapted from Calado *et al.*[1]

**Source and Purity of Materials:**
(1) Aldrich Chemical Inc.; purity 96.0 mass %; dried and double distilled under a reduced pressure in a 36 in. glass column; purity 99.96–99.98 mass %.
(2) Aldrich Chemical Inc.; research grade; purity 96.0 mass %; distilled at atmospheric pressure in the 36 in. glass column; purity 99.99 mass % by GLC.

**Estimated Error:**
Not specified.

**References:**
[1]J. C. G. Calado, I. A. McLure, and V. A. M. Soares, Fluid Phase Equilib. **2**, 199 (1978).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
H. Tanaka and Y. Wada, Chem. Phys. **78**, 143–9 (1983).

**Variables:**
$T$/K = 299

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The upper critical solution temperature was reported to be 25.94 °C (299.09 K) at 100 $w_1$ = 46.56 ($x_1$ = 0.5000, compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
These data are from a study of the adiabatic compressibility of (1) and (2) critical mixture. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; commercial reagent of extra pure grade; purified by the use of molecular sieves.
(2) Source not specified; commercial reagent of extra pure grade; used without further purification.

**Estimated Error:**
Temperature: ±0.005 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 3-Methylpentane; $C_6H_{14}$ ; [96-14-0]

**Original Measurements:**
I. L. Pegg and I. A. McLure, Mol. Phys. **53**, 897–916 (1984).

**Variables:**
$T$/K = 293–300

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Shear viscosities and densities of the equilibrium liquid phases of the nitroethane (1)+3-methylpentane (2) system

| $t$/°C | $T$/K (compilers) | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| | | $\rho$(g·L$^{-1}$) | $\eta$(cP) | $\rho$(g·L$^{-1}$) | $\eta$(cP) |
| 19.450 | 292.600 | 714.6 | 0.3411 | 906.2 | 0.5251 |
| 21.450 | 294.600 | 719.9 | 0.3424 | 891.7 | 0.5051 |
| 22.450 | 295.600 | 723.5 | 0.3447 | 883.4 | 0.4948 |
| 23.450 | 296.600 | 728.3 | 0.3483 | 874.0 | 0.4849 |
| 24.450 | 297.600 | 735.0 | 0.3549 | 862.8 | 0.4747 |
| 25.450 | 298.600 | 745.5 | 0.3686 | 847.7 | 0.4662 |
| 26.150 | 299.300 | 760.4 | 0.3971 | 829.6 | 0.4655 |
| 26.400 | 299.550 | 775.0 | 0.4395 | 813.8 | 0.4810 |
| 26.440 | 299.590 | 782.8 | 0.4663 | 805.8 | 0.4950 |
| 26.450 | 299.600 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Capillary flow viscosimetry was used. Ubbelhode type viscometer was modified to measure viscosity of coexisting liquid phases. The viscometer and stirrer were placed in a bath having a temperature measured with a precision of 1 mK, using a Pt resistance thermometer. CST for each sample was determined visually, on repeated heating and cooling.

**Source and Purity of Materials:**
(1) Fisons; purity 95.0 mass %; fractionally distilled on a spinning band column at reduced pressure; purity 99.97 mass %.
(2) Koch-Light; puriss; 3 mass % of 2-methyl-pentane impurity; fractionated on a spinning band column; 0.01 mass % organic impurities by GLC.

**Estimated Error:**
Temperature: control to ±0.001 K.

## 3.9. Hexane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system nitroethane+hexane were reported in the publications listed in Table 1.

Table 1. Summary of solubility data for the system nitroethane+hexane

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Hwa *et al.*[1] | 276–302 | mutual | analytical/synthetic |
| Clever *et al.*[2] | 289–306 | mutual | synthetic |
| Snyder and Eckert[3] | 301–305 | mutual | synthetic |
| Hsu and Clever[4] | 298 | mutual | not stated |
| Beridze and Karshibaev[5] | 304 | UCST | not stated |
| Ziolo *et al.*[6] | 289–301 | mutual | not stated |

All original data are given in the data sheets immediately following this Critical Evaluation. The following individual points in otherwise satisfactory studies are in marked disagreement with other studies and have been rejected: in the nitroethane-rich phase at 298 K (Snyder and Eckert[3]), 301.5 and 302.4 K.[1] Table 2 has been prepared on the basis of all other reported data.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in the Table 2. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of nitroethane (1) and hexane (2)

| | Hexane-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|
| $T$/K | $100\,w_1$ | $x_1$ | | $100\,w_2$ | $x_2$ | |
| 278.2 | 8.8 | 0.100 | tentative | 11.0 | 0.097 | tentative |
| 283.2 | 10.8 | 0.123 | tentative | 13.8 | 0.116 | tentative |
| 288.2 | 13.6 | 0.153 | tentative | 18.8 | 0.168 | recommended |
| 293.2 | 18.2 | 0.203 | tentative | 22.0 | 0.197 | recommended |
| 298.2 | 23.9 | 0.265 | recommended | 27.4 | 0.247 | recommended |
| 301.2 | 28.6 | 0.315 | tentative | 31.0 | 0.281 | recommended |
| 303.2 | 30.4 | 0.334 | tentative | 35.0 | 0.319 | recommended |
| 304.2 | 34.2 | 0.374 | tentative | 38.2 | 0.350 | recommended |

The upper critical solution temperature has been reported as 300.575 K,[6] 302.5 K,[1] 304.1 K,[5] 304.5 K,[3] and 305.7 K.[2] Thus, the tentative value is: $T_c$=(303.5±2) K. The corresponding critical solution composition has been reported as $x_{c1}$=0.500 (Beridze and Karshibaev[5]) and $x_{c1}$=0.560.[6] Thus, the tentative value is: $x_{c1}$=0.53±0.03.

The recommended and tentative values for the mutual solubility reported in the above table were approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived: $a_1$=0.82346, $a_2$=0.31876, $b_1$=4.24293, $b_2$=−3.51701 (mean standard error of estimate was 0.0359).

For this approximation, the tentative values of UCST and $x_{c1}$ have been used. This relationship is presented in Fig. 5 together with experimental data reported in four references.[1–3,6]

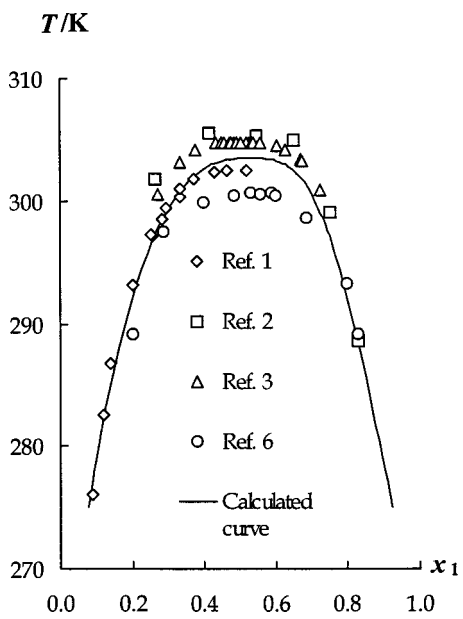


FIG. 5. Mutual solubility of nitroethane and hexane.

**References:**
[1]S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409 (1963).
[2]H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31 (1972).
[3]R. B. Snyder and C. A. Eckert, J. Chem. Eng. Data **18**, 282 (1973).
[4]K. Y. Hsu and H. L. Clever, J. Chem. Eng. Data **20**, 268 (1975).
[5]D. K. Beridze and A. K. Karshibaev, Fizika i fiziko-khimiaj zhidkostei. Moskva **3**, 138 (1976).
[6]J. Ziolo, Z. Ziejewska, and J. Piotrowska, J. Phys. Chem. **84**, 979 (1980).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 276–302

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and hexane (2)

| | | Hexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 2.90 | 276.05 | 7.9 | 0.090 | 89.9 | 0.911 |
| 9.40 | 282.55 | 10.6 | 0.120 | 86.4 | 0.879 |
| 13.65 | 286.80 | 12.4 | 0.140 | ··· | ··· |
| 19.95 | 293.10 | 18.2 | 0.203 | 78.6 | 0.808 |
| 24.00 | 297.15 | 23.1 | 0.256 | 73.5 | 0.761 |
| 24.1[a] | 297.25 | 22.63 | 0.251 | ··· | ··· |
| 25.30 | 298.45 | 25.7 | 0.284 | 71.0 | 0.738 |
| 26.1[a] | 299.25 | ··· | ··· | 68.42 | 0.713 |
| 26.25 | 299.40 | 26.6 | 0.294 | 69.0 | 0.719 |
| 27.20 | 300.35 | 30.2 | 0.332 | 67.6 | 0.706 |
| 27.4[a] | 300.55 | ··· | ··· | 65.13 | 0.682 |
| 27.8[a] | 300.95 | 30.5 | 0.335 | ··· | ··· |
| 28.3[a] | 301.45 | ··· | ··· | 61.63 | 0.648 |
| 28.7[a] | 301.85 | 33.9 | 0.371 | ··· | ··· |
| 29.2[a] | 302.35 | 39.83 | 0.432 | 54.45 | 0.579 |
| 29.3[a] | 302.45 | 42.97 | 0.464 | 48.48 | 0.519 |
| 29.30 | 302.45 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to ±0.1 K (synthetic method),
Composition: ±0.5 mass % (analytical method).

**References:**
[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 289–306

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and hexane (2)

| | | Hexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | 100 $w_1$ (compilers) | $x_1$ | 100 $w_1$ (compilers) |
| 15.4 | 288.6 | ··· | ··· | 0.830 | 81.0 |
| 25.4 | 299.1 | ··· | ··· | 0.750 | 72.3 |
| 28.6 | 301.8 | 0.265 | 23.9 | ··· | ··· |
| 31.8 | 305.0 | ··· | ··· | 0.650 | 61.8 |
| 32.1 | 305.3 | ··· | ··· | 0.545 | 51.1 |
| 32.4 | 305.6 | ··· | ··· | 0.415 | 38.2 |
| 32.5 | 305.7 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solutions of (1) and (2) were prepared by weight from glass syringes in 13 mm×100 mm Kimax screw cap culture tubes and sealed by a cap with a Teflon faced rubber liner. The tubes were suspended in a 3 L well-stirred water bath and cloud points observed visually. At least two observations were made of each set of samples: the first at a relatively fast cooling rate to find the approximate cloud point temperature and the second at a slow cooling rate to more precisely determine the cloud point temperature.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled at 57 °C/12.9 kPa.
(2) Phillips; purity 99 mole %.

**Estimated Error:**
Temperature: control to ±0.1 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
R. B. Snyder and C. A. Eckert, J. Chem. Eng. Data **18**, 282–5 (1973).

**Variables:**
$T$/K = 301–305

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and hexane (2)

| | | Hexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | 100 $w_1$ (compilers) | $x_1$ | 100 $w_1$ (compilers) |
| 27.35 | 300.50 | 0.271 | 24.46 | ··· | ··· |
| 27.71 | 300.86 | ··· | ··· | 0.723 | 69.45 |
| 30.01 | 303.16 | 0.334 | 30.40 | ··· | ··· |
| 30.07 | 303.22 | ··· | ··· | 0.676 | 64.50 |
| 30.19 | 303.34 | ··· | ··· | 0.671 | 63.98 |
| 31.04 | 304.19 | 0.377 | 34.51 | ··· | ··· |
| 31.09 | 304.24 | ··· | ··· | 0.626 | 59.31 |
| 31.41 | 304.56 | ··· | ··· | 0.606 | 57.26 |
| 31.59 | 304.74 | 0.435 | 40.14 | 0.558 | 52.43 |
| 31.60 | 304.75 | 0.448 | 41.41 | 0.540 | 50.55 |
| 31.60 | 304.75 | ··· | ··· | 0.534 | 49.95 |
| 31.61 | 304.76 | 0.456 | 42.20 | 0.505 | 47.05 |
| 31.61 | 304.76 | 0.471 | 43.68 | 0.491 | 45.66 |
| 31.62 | 304.77 | 0.485 | 45.06 | 0.520 | 48.55 |
| 31.63 | 304.78 | 0.478 | 44.37 | 0.527 | 49.25 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubility temperatures were determined from a set of samples made up to composition by weight and sealed into 7 mm Pyrex tubes about 9 cm long. A short length of glass rod was placed in each tube as a stirrer. An apparatus was constructed to rotate the tube end over end inside the temperature bath, so that the glass rod stirrer would fall through the liquid, causing mixing. The apparatus consisted of a submerged horizontal drive shaft with a fuse holder perpendicularly attached to one end. The sealed glass tube was placed on the fuse holder, and the shaft was rotated by a rubber pulley connected to a 4 rpm electric motor mounted on a platform above the water level.

**Source and Purity of Materials:**
(1) Source not specified; distilled in 1.5 m column packed with nichrome helices; purity 99.9 mass %.
(2) Source not specified; distilled at a 15:1 reflux ratio in 1 m column packed with glass helices; boiling point = 68.8 °C–69.1 °C.

**Estimated Error:**
Temperature: control to ±0.1 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
K.-Y. Hsu and H. L. Clever, J. Chem. Eng. Data **20**, 268–71 (1975).

**Variables:**
$T$/K = 298

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The mole fraction of nitroethane in the (2)-rich phase at equilibrium at 298 K was reported to be $x_1 = 0.2540$, corresponding 100 $w_1 = 22.87$ (compiler).

The mole fraction of nitroethane in the (1)-rich phase at equilibrium at 298 K was reported to be $x_1 = 0.7815$, corresponding 100 $w_1 = 75.70$ (compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
These data are from a study of the enthalpy of mixing of (1) and (2) by microflow calorimetry. No experimental details given.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled; boiling point = 57 °C/12.9 kPa, $n$(25 °C,D) = 1.389 50.
(3) Fisher; distilled from over $CaH_2$; $n$(25 °C,D) = 1.372 40, $\rho$(30 °C) = 650.38 g·L$^{-1}$.

**Estimated Error:**
Temperature: control to ±0.02 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
D. K. Beridze and A. K. Karshibaev, Fizika i fiziko-khimiya zhidkostei, Moskva **3**, 138–51 (1976).

**Variables:**
$T$/K = 304

**Prepared By:**
N. I. Lisov

**Experimental Data**

The upper critical solution temperature was reported to be 30.95 °C (304.10 K, compiler) at $x_1 = 0.50$ (100 $w_1 = 46.6$, compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; distilled; boiling point = 81.5–82.0 °C/35.1 kPa; $n$(20 °C,D) = 1.3920; $\rho$(20 °C) = 1052 g·L$^{-1}$.
(2) Source not specified; purity not specified; distilled; boiling point = 68.7 °C; $n$(20 °C,D) = 1.3748.

**Estimated Error:**
Composition: ±0.1 mole %.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**
J. Ziolo, Z. Ziejewska, and J. Piotrowska, J. Phys. Chem. **84**, 979–80 (1980).

**Variables:**
$T$/K = 289–301

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual of solubility of nitromethane (1) and hexane (2) in mole fractions terms were reported over the temperature range in graphical form. The data table was extracted by the compilers from the published graphs.

Mutual solubility of nitroethane (1) and hexane (2)

| | | Hexane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | 100 $w_1$ (compilers) | $x_1$ | 100 $w_1$ (compilers) |
| 15.3 | 288.5 | ··· | ··· | 0.828 | 80.7 |
| 16.0 | 289.2 | 0.200 | 17.9 | ··· | ··· |
| 20.1 | 293.3 | ··· | ··· | 0.800 | 77.7 |
| 24.3 | 297.5 | 0.288 | 26.1 | ··· | ··· |
| 25.4 | 298.6 | ··· | ··· | 0.686 | 65.6 |
| 26.7 | 299.9 | 0.400 | 36.7 | ··· | ··· |
| 27.2 | 300.4 | 0.486 | 45.2 | 0.600 | 56.6 |
| 27.4 | 300.6 | 0.531 | 49.7 | 0.590 | 55.6 |
| 27.425 | 300.575 | 0.560 | 52.6 | 0.560 | 52.6 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.

**Estimated Error:**
Not reported.

## 3.10. Methylcyclohexane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Methylcyclohexane; $C_7H_{14}$ ; [108-87-2]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

### Critical Evaluation

Solubilities in the system nitroethane (1)+methylcyclohexane (2) were reported in three publications. Francis[1] determined the upper critical solution temperature. Clever *et al.*[2] measured the mutual solubilities of the two components between 282 and 298 K by the synthetic method. Pyzuk *et al.*[3] determined the upper critical solution temperature by the synthetic method and the critical solution composition.

The upper critical solution temperature has been reported as 294.5 K,[1] 295.2 K,[3] and 298.2 K.[2] The corresponding critical solution composition has been reported as $\varnothing^*_{c1}=0.346$, $x_{c1}=0.486$.[2] The experimental data reported in Clever *et al.*[2] and Pyzuk *et al.*[3] have been approximated (with the same weighing factor) by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1=0.767\,90,\ a_2=0.640\,79,\ b_1=-2.481\,27,\ b_2=1.784\,00\ \text{(mean standard error of estimate was 0.0183)}.$$

For this approximation UCST and $x_{c1}$ from Clever *et al.*[2] and Pyzuk *et al.*[3] were used, respectively. In the opinion of the evaluator, the smoothed mutual solubilities, calculated by this equation, may be treated as tentative. The results of calculations for the selected temperatures are presented in the following table. This relationship together with experimental points (Clever *et al.*[2]) are also presented in Fig. 6.

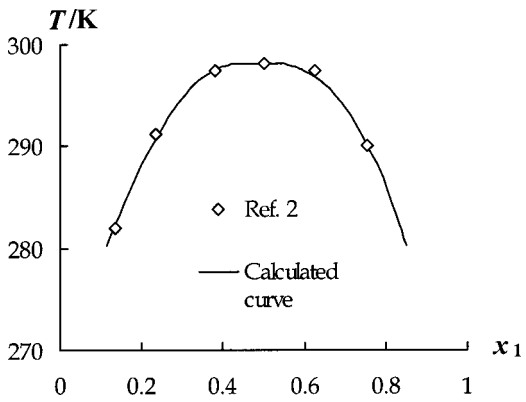


FIG. 6. Mutual solubility of nitroethane and methylcyclohexane.

Mutual solubility of nitroethane and methylcyclohexane

| | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|
| $T$/K | $x_1$ | 100 $w_1$ | $x_1$ | 100 $w_1$ |
| 283.2 | 0.145 | 11.5 | 0.827 | 78.5 |
| 288.2 | 0.200 | 16.0 | 0.779 | 72.9 |
| 293.2 | 0.270 | 22.0 | 0.713 | 65.5 |
| 294.2 | 0.287 | 23.5 | 0.695 | 63.5 |
| 295.2 | 0.308 | 25.4 | 0.674 | 61.3 |
| 296.2 | 0.332 | 27.5 | 0.648 | 58.5 |
| 297.2 | 0.365 | 30.5 | 0.612 | 54.7 |
| 297.5 | 0.379 | 31.8 | 0.597 | 53.1 |
| 297.6 | 0.385 | 32.4 | 0.591 | 52.5 |
| 297.7 | 0.391 | 32.9 | 0.585 | 51.9 |
| 297.8 | 0.398 | 33.6 | 0.577 | 51.0 |
| 297.9 | 0.406 | 34.3 | 0.569 | 50.2 |
| 298.0 | 0.416 | 35.3 | 0.558 | 49.1 |

*∅- volume fraction.

**References:**

[1]A. W. Francis, ''Critical Solution Temperature,'' Adv. Chem. Ser. **31** (1961).
[2]H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31 (1972).
[3]W. Pyzuk, T. Krupkowski, J. Dolecki, and B. Paduszek, Pol. J. Chem. **56**, 1477 (1982).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Methylcyclohexane; $C_7H_{14}$; [108-87-2]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 282–298

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and methylcyclohexane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | 100 $w_1$ (compilers) | $x_1$ | 100 $w_1$ (compilers) |
| 8.8 | 282.0 | 0.135 | 10.7 | ··· | ··· |
| 16.9 | 290.1 | ··· | ··· | 0.755 | 70.2 |
| 18.0 | 291.2 | 0.235 | 19.0 | ··· | ··· |
| 24.2 | 297.4 | ··· | ··· | 0.625 | 56.0 |
| 24.3 | 297.5 | 0.380 | 31.9 | ··· | ··· |
| 24.9 | 298.1 | ··· | ··· | 0.500 | 43.3 |
| 25.0 | 298.2 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solutions of (1) and (2) were prepared by weight from glass syringes in 13–100 mm Kimax screw cap culture tubes and sealed by a cap with a Teflon faced rubber liner. The tubes were suspended in a 3 L well-stirred water bath and cloud points observed visually. At least two observations were made of each set of samples: the first at a relatively fast cooling rate to find the approximate cloud point temperature and the second at a slow cooling rate to more precisely determine the cloud point temperature.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled at 57 °C/12.9 kPa.
(2) Phillips; purity 99 mole %; shaken with concentrated $H_2SO_4$; washed with water; dried over $CaSO_4$ and distilled at atmospheric pressure from $CaH_2$.

**Estimated Error:**
Temperature: control to ±0.1 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Methylcyclohexane; $C_7H_{14}$; [108-87-2]

**Original Measurements:**
W. Pyzuk, T. Krupkowski, J. Dolecki, and B. Paduszek, Pol. J. Chem. **56**, 1477–82 (1982).

**Variables:**
$T$/K = 295

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
The solubility temperatures of nitroethane (1) and methylcyclohexane (2) were determined for 22 mixtures, but these data are not given in the original publication.

Upper critical solution temperature was reported to be 295.2 K at $\varnothing_1 = 0.346$ (100 $w_1 = 42.0$ and $x_1 = 0.486$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method described in Pyzuk[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; treated with sulfuric acid, washed, dried and distilled under reduced pressure over Sikkon; about 2.5 mass % of nitropropane impurity.
(2) Fluka; not specified.

**Estimated Error:**
Not specified.

**References:**
[1]W. Pyzuk, Chem. Phys. **50**, 281 (1980).

## 3.11. Heptane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Heptane; $C_7H_{16}$ ; [142-82-5]

**Original Measurements:**
E. G. Komarova, and V. B. Kogan, Zh. Prikl. Khim. (Leningrad) **37**, 1776–86 (1964).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

### Experimental Data

The mole fraction of nitroethane in the (2)-rich phase at equilibrium at 293.2 K was reported to be $x_1 = 0.1711$, corresponding $100\,w_1 = 11.17$ (compiler).

The mole fraction of nitroethane in the (1)-rich phase at equilibrium at 293.2 K was reported to be $x_1 = 0.8695$, corresponding $100\,w_1 = 80.23$ (compiler).

### Auxiliary Information

**Method/Apparatus/Procedure:**
The analytical method was used. A mixture of (1) and (2) was placed in a thermostated cell and stirred for 1 h. The compositions of the phases were determined by gas chromatography.

**Source and Purity of Materials:**
(1) Distilled in 1.2 m packed fractionating column; boiling point = 114 °C; $n$(20 °C,D) = 1.3920; $d$(20 °C,4 °C) = 1.0520.
(2) Distilled in 1.2 m packed fractionating column; boiling point = 98.4 °C; $n$(20 °C,D) = 1.3877.

**Estimated Error:**
Temperature: control to ±0.1 K.

## 3.12. 1-Octene

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Octene; $C_8H_{16}$ ; [111-66-0]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 246–269

**Prepared By:**
N. I. Lisov and V. P. Sazonov

### Experimental Data

Mutual solubility of nitroethane (1) and 1-octene (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $100\,w_1$ | $x_1$ (compilers) | $100\,w_1$ | $x_1$ (compilers) |
| −27.5 | 245.7 | 8.5 | 0.122 | 86.8 | 0.908 |
| −25.4 | 247.8 | 9.6 | 0.137 | 86.0 | 0.902 |
| −21.6 | 251.6 | 11.5 | 0.163 | 83.8 | 0.885 |
| −19.7 | 253.5 | 12.5 | 0.176 | 82.6 | 0.876 |
| −16.7 | 256.5 | 14.9 | 0.207 | 80.1 | 0.857 |
| −13.0 | 260.2 | 18.3 | 0.251 | 76.5 | 0.830 |
| −11.0 | 262.2 | 20.9 | 0.283 | 73.9 | 0.809 |
| −9.0 | 264.2 | 23.5 | 0.315 | 70.7 | 0.783 |
| −7.8 | 265.4 | 26.2 | 0.347 | 68.8 | 0.767 |
| −6.5[a] | 266.7 | ··· | ··· | 63.5 | 0.722 |
| −5.8[a] | 267.4 | 30.99 | 0.402 | ··· | ··· |
| −4.7[a] | 268.5 | ··· | ··· | 54.97 | 0.646 |
| −4.7[a] | 268.5 | ··· | ··· | 49.91 | 0.598 |
| −4.6[a] | 268.6 | 41.16 | 0.511 | ··· | ··· |
| −4.6 | 268.6 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to 0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**
[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

## 3.13. Octanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Octanoic acid; $C_8H_{16}O_2$; [124-07-2]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K=273 and 283

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Solubility of octanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 25.2 | 20.1 | 0.116 |
| 10.0 | 283.2 | 790 | 88.8 | 0.804 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*,[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*[1] (dried and twice distilled).
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=16.3 °C.

**Estimated Error:**
Not reported.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.14. Octanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Octanamide; $C_8H_{17}NO$; [629-01-6]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K=283–373

**Prepared By:**
V. P. Sazonov; N. I. Lisov, and N. V. Sazonov

**Experimental Data**

The solubilities of octanamide (2) in nitroethane (1) in mass percent over the temperature range were reported in graphical form and in a table.

Solubility of octanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 1.0 | 1.0 | 0.005 |
| 16.8* | 290.0 | ··· | 1.4 | 0.007 |
| 30.0 | 303.2 | 2.1 | 2.1 | 0.011 |
| 32.7* | 305.9 | ··· | 2.5 | 0.013 |
| 46.4* | 319.6 | ··· | 5.6 | 0.030 |
| 50.0 | 323.2 | 7.5 | 7.0 | 0.038 |
| 60.9* | 334.1 | ··· | 14.1 | 0.079 |
| 70.0 | 343.2 | 37.5 | 27.3 | 0.164 |
| 73.8* | 347.0 | ··· | 34.5 | 0.216 |
| 79.1* | 352.3 | ··· | 47.3 | 0.320 |
| 82.7* | 355.9 | ··· | 56.6 | 0.406 |
| 86.8* | 360.0 | ··· | 67.1 | 0.517 |
| 90.0 | 363.2 | 307 | 75.4 | 0.617 |
| 92.7* | 365.9 | ··· | 81.8 | 0.702 |
| 96.4* | 369.6 | ··· | 89.1 | 0.811 |
| 99.1* | 372.3 | ··· | 92.5 | 0.866 |
| 100.0 | 373.2 | 1600 | 94.1 | 0.894 |

*These data are extracted by compilers from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the octanoic acid at 190–210 °C for 10–14 h; purified by recrystallization; freezing point=105.9 °C.

**Estimated Error:**
Temperature: control to ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.15. 2,2,4-Trimethylpentane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system nitroethane (1) +2,2,4-trimethylpentane (2) were reported in the publications listed in Table 1.

Table1. Summary of solubility data for the system nitroethane +2,2,4-trimethylpentane

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Vreeland and Dunlap[1] | 298–303 | mutual | synthetic |
| Hwa *et al.*[2] | 275–303 | mutual | analytical/synthetic |
| Hsu and Clever[3] | 298 | mutual | not stated |
| Beysens[4] | 297–304 | mutual | synthetic |
| Tanaka and Wada[5] | 303 | UCST | not stated |
| Battler and Rowley[6] | 293 and 302 | mutual | not stated |

Beysens and Tufeu[7] determined of the variation of the critical temperature as a function of pressure (from 500 to 12 500 kPa). All original data are compiled immediately following this Critical Evaluation.

The data point for the nitroethane-rich phase at 298 K (Hsu and Clever[3]) is marked disagreement with other studies and is therefore rejected. Table 2 has been prepared on the basis of all other reported data. Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in Table 2. Data are "recommended" if two or more apparently reliable studies are reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of nitroethane and 2,2,4-trimethylpentane

| | Hydrocarbon-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|
| $T$/K | 100 $w_1$ | $x_1$ | | 100 $w_2$ | $x_2$ | |
| 278.2 | 8.7 | 0.126 | tentative | 14.5 | 0.100 | tentative |
| 283.2 | 10.7 | 0.155 | tentative | 16.6 | 0.115 | tentative |
| 288.2 | 13.2 | 0.188 | tentative | 19.5 | 0.137 | tentative |
| 293.2 | 15.3 | 0.212 | tentative | 23.4 | 0.167 | recommended |
| 298.2 | 22.3 | 0.304 | recommended | 28.7 | 0.209 | recommended |
| 300.2 | 28.9 | 0.382 | recommended | 31.8 | 0.234 | recommended |
| 302.2 | 33.3 | 0.432 | recommended | 38.2 | 0.288 | recommended |

The upper critical solution temperature (USCT) has been reported as 302.15 K,[6] 302.7 K,[2] 303.0 K,[1] 303.18 K,[4] and 303.20 K.[5] The UCST of Battler and Rowley[6] is rejected. Thus, the recommended value is: $T_c$=303.0±0.2 K.

The corresponding critical solution composition has been reported as $x_{c1}$ = 0.491 (Vreeland and Dunlap[1]), $x_{c1}$ = 0.569 (Beysens[4]), and $x_{c1}$ = 0.5692 (Tanaka and Wada[5]). The $x_{c1}$ of Vreeland and Dunlap[1] is rejected. The data average $x_{c1}$ = 0.569. This value is recommended.

The recommended and tentative values for the mutual solubility reported in Table 2 have been approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived: $a_1$ = 0.958 70, $a_2$ = − 0.243 93, $b_1$ = 1.50442, $b_2$ = 1.689 14 (mean standard error of estimate was 0.0118).

For this approximation, recommended values of UCST and $x_{c1}$ have been used. This relationship is presented in Fig. 7 together with experimental data reported in several references.[1,2,4]

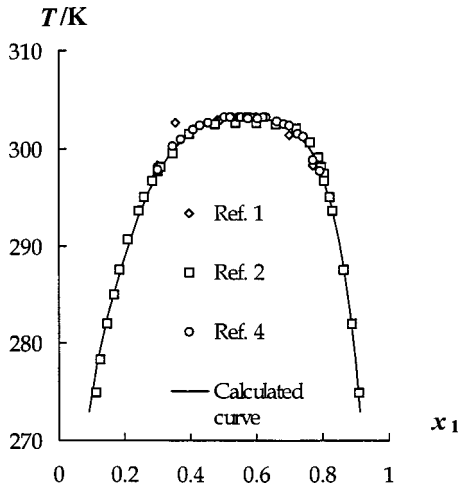


FIG. 7. Mutual solubility of nitroethane and 2,2,4-trimethylpentane.

**References:**
[1]J. Vreeland and R. Dunlap, J. Phys. Chem. **62**, 329 (1957).
[2]S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409 (1963).
[3]K.-Y. Hsu and H. L. Clever, J. Chem. Eng. Data **20**, 268 (1975).
[4]D. Beysens, J. Chem. Phys. **71**, 2557 (1979).
[5]H. Tanaka and Y. Wada, Chem. Phys. **78**, 143 (1983).
[6]J. R. Battler and R. L. Rowley, J. Chem. Eng. Data **35**, 334 (1990).
[7]D. Beysens and R. Tufeu, Rev. Phys. Appl. **14**, 907 (1979).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
J. Vreeland and R. Dunlap, J. Phys. Chem. **61**, 329–33 (1957).

**Variables:**
$T$/K = 298–303

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual solubility of nitromethane (1) and 2,2,4-trimethylpentane (2) in mass fractions were reported over the temperature range in graphical form. The compilers extracted the data presented in this table from the published graphs.

Mutual solubility of nitroethane (1) and 2,2,4-trimethylpentene (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 25.0 | 298.2 | 22.0 | 0.300 | 68.9 | 0.771 |
| 28.2 | 301.4 | ··· | ··· | 60.4 | 0.699 |
| 29.5 | 302.7 | 26.4 | 0.353 | ··· | ··· |
| 29.7 | 302.9 | 37.9 | 0.482 | 43.3 | 0.538 |
| 29.8 | 303.0 | 38.8 | 0.491 | 38.8 | 0.491 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solutions of known composition were heated above the critical solution temperature and placed in a bath, which was cooled at the rate of 0.01 K/min. The solutions were agitated and the temperature at which phase separation occurred was observed.

**Source and Purity of Materials:**
(1) Matheson, Chemical Co; research grade; distilled through a Todd column; boiling point = 114.7–114.8 °C.
(2) Phillips Petroleum Co.; 99 mole % purity; $\rho$(25 °C) = 687.74 $g \cdot L^{-1}$.

**Estimated Error:**
Temperature: control to ±0.02 K;
Solubility: 1%.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 275–303

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Mutual solubility of nitroethane (1) and 2,2,4-timethylpentane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 1.80 | 274.95 | 7.7 | 0.113 | 86.6 | 0.908 |
| 5.12 | 278.27 | 8.7 | 0.127 | ··· | ··· |
| 8.80 | 281.95 | 10.2 | 0.147 | 83.9 | 0.888 |
| 11.90 | 285.05 | 11.5 | 0.165 | ··· | ··· |
| 14.40 | 287.55 | 13.0 | 0.185 | 80.7 | 0.864 |
| 17.42 | 290.57 | 14.9 | 0.210 | ··· | ··· |
| 20.45 | 293.60 | 17.4 | 0.243 | 76.4 | 0.831 |
| 21.85 | 295.00 | 18.6 | 0.258 | 75.2 | 0.822 |
| 23.63 | 296.78 | 20.7 | 0.284 | 73.2 | 0.806 |
| 24.2[a] | 297.35 | ··· | ··· | 72.79 | 0.803 |
| 24.6[a] | 297.75 | 22.08 | 0.301 | ··· | ··· |
| 25.01 | 298.16 | 22.60 | 0.308 | 72.1 | 0.797 |
| 26.0[a] | 299.15 | ··· | ··· | 70.9 | 0.788 |
| 26.4[a] | 299.55 | 25.89 | 0.347 | ··· | ··· |
| 27.5[a] | 300.65 | ··· | ··· | 67.99 | 0.764 |
| 28.3[a] | 301.45 | 30.15 | 0.396 | ··· | ··· |
| 28.9[a] | 302.05 | ··· | ··· | 62.89 | 0.721 |
| 29.4[a] | 302.55 | 37.52 | 0.477 | 55.88 | 0.658 |
| 29.5[a] | 302.65 | 43.11 | 0.536 | 49.49 | 0.599 |
| 29.5 | 302.65 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to 0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**
[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
K.-Y. Hsu and H. L. Clever, J. Chem. Eng. Data **20**, 268–71 (1975).

**Variables:**
$T$/K = 298

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The mole fraction of nitroethane in the (2)-rich phase at equilibrium at 298.2 K was reported to be $x_1 = 0.3008$, corresponding $100\ w_1 = 22.04$ (compiler).

The mole fraction of nitroethane in the (1)-rich phase at equilibrium at 298.2 K was reported to be $x_1 = 0.8186$, corresponding $100\ w_1 = 74.79$ (compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled; boiling point = 57 °C/12.9 kPa; $n$(25°C,D) = 1.3895; $\rho$(30 °C) = 1034.5 g·L$^{-1}$.
(2) Phillips; research grade; $n$(25 °C,D) = 1.389 05; $\rho$(30 °C) = 683.44 g·L$^{-1}$.

**Estimated Error:**
Temperature: control to ±0.02 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
D. Beysens, J. Chem. Phys. **71**, 2557–65 (1979).

**Variables:**
$T$/K = 298–303

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Mutual solubility of nitroethane (1) and 2,2,4-trimethylpentene (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 24.490 | 297.640 | ··· | ··· | 71.5 | 0.792 |
| 24.734 | 297.884 | 22.0 | 0.300 | ··· | ··· |
| 25.630 | 298.780 | ··· | ··· | 69.0 | 0.772 |
| 27.030 | 300.180 | 25.7 | 0.345 | ··· | ··· |
| 27.770 | 300.920 | 28.0 | 0.372 | ··· | ··· |
| 28.054 | 301.204 | ··· | ··· | 65.2 | 0.740 |
| 28.321 | 301.471 | ··· | ··· | 63.4 | 0.725 |
| 28.795 | 301.945 | 31.1 | 0.407 | ··· | ··· |
| 29.197 | 302.347 | ··· | ··· | 60.8 | 0.702 |
| 29.234 | 302.384 | 33.0 | 0.428 | ··· | ··· |
| 29.404 | 302.554 | ··· | ··· | 58.8 | 0.685 |
| 29.513 | 302.663 | 35.4 | 0.455 | ··· | ··· |
| 29.707 | 302.857 | ··· | ··· | 56.5 | 0.664 |
| 29.951 | 303.101 | ··· | ··· | 47.3 | 0.577 |
| 29.960 | 303.110 | ··· | ··· | 50.1 | 0.604 |
| 29.996 | 303.146 | 46.0 | 0.565 | ··· | ··· |
| 30.005 | 303.155 | ··· | ··· | 48.1 | 0.585 |
| 30.008 | 303.158 | 44.0 | 0.545 | ··· | ··· |
| 30.009 | 303.159 | ··· | ··· | 52.0 | 0.622 |
| 30.011 | 303.161 | 40.0 | 0.504 | ··· | ··· |
| 30.013 | 303.163 | 44.8 | 0.553 | ··· | ··· |
| 30.014 | 303.164 | ··· | ··· | 47.0 | 0.574 |
| 30.017 | 303.167 | 42.1 | 0.525 | ··· | ··· |
| 30.035 | 303.185 | ··· | ··· | 49.5 | 0.599 |
| 30.058 | 303.208 | ··· | ··· | 52.8 | 0.630 |
| 30.067 | 303.217 | 41.8 | 0.522 | ··· | ··· |
| 30.081 | 303.231 | ··· | ··· | 49.7 | 0.601 |
| 30.030 | 303.180 | 46.5 | 0.569 | 46.5 | 0.569 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The visual method was used. Dried Pyrex cells, 3 cm high, contained the weighed mixture. When filled and shut, cells were frozen in liquid nitrogen and sealed under vacuum. Samples were immersed in a large water bath where they could be seen through a double window. Thermal stabilization was $>10^{-3}$ K (verified by Pt resistance thermometer and a Smith bridge). The sample was shaken, heated, introduced into the bath; if a meniscus was visible, the bath temperature was increased and operation repeated; if not visible, bath temperature was lowered while shaking the sample.

**Source and Purity of Materials:**
(1) Source not specified; 96% pure commercial material; purity by distillation; 0.5 mass % impurity by gas chromatography; $\rho$(30 °C) = 1040.4 g·L$^{-1}$.
(2) Source not specified; reagent for chromatography; $\rho$(30 °C) = 693.7 g·L$^{-1}$.

**Estimated Error:**
Temperature: to ±0.001 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
D. Beysens and R. Tufeu, Rev. Phys. Appl. **14**, 907–9 (1979).

**Variables:**
$T$/K = 303–304; $P$/kPa = 500–12 500

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The variation of the critical temperature as a function of pressure in the critical mixture of (1) and (2) over the temperature and pressure range was presented in a graphical form in the original publication. The compiler extracted the numerical data in the table below graphically.

Effect of pressure on solubility of mixture nitroethane (1) and 2,2,4-trimethylpentane (2)

| 100 $w_1$ | $x_1$ (compiler) | $P$/kPa | Solubility temperatures, $T$/K: Experiment | Solubility temperatures, $T$/K: Avg. (compiler) | $t$/°C (compiler) |
|---|---|---|---|---|---|
| 46.9 | 0.573 | 500 | 303.29; 303.31; 303.35 | 303.32 | 30.17 |
| | | 1250 | 303.35 | 303.35 | 30.20 |
| | | 2500 | 303.21; 303.28 | 303.25 | 30.10 |
| | | 5000 | 303.26; 303.30 | 303.28 | 30.13 |
| | | 7500 | 303.45 | 303.45 | 30.30 |
| | | 10 000 | 303.53; 303.54 | 303.54 | 30.39 |
| | | 12 500 | 303.64 | 303.64 | 30.49 |

A value of $dT_c/dP$ of $(2.6 \pm 0.5) \cdot 10^{-8}$ K·Pa$^{-1}$ was reported in the above pressure range.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Heating as glass tube and varying the pressure mixed the mixture; then the thermostat was set at a temperature high enough so that the mixture remained in the one phase region when the desired pressure was applied. When thermal equilibrium was reached, the temperature was lowered. Another equilibrium takes place and an observation was done in order to detect the meniscus. If it is not visible, another step was performed.

**Source and Purity of Materials:**
(1) Source not specified; purity 96.0 mass %; distilled; the impurity level less than 0.5 mass % by gas chromatography and nuclear magnetic resonance (NMR).
(2) Source not specified; reagent for gas chromatography; not purified.

**Estimated Error:**
Temperature: ±0.01 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
H. Tanaka and Y. Wada, Chem. Phys. **78**, 143–9 (1983).

**Variables:**
$T$/K = 303

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The upper critical solution temperature was reported to be 30.05 °C (303.20 K) at 100 $w_1$ = 46.48 ($x_1$ = 0.5693, compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; commercial reagent of extra pure grade; purified by the use of molecular sieves.
(2) Commercial reagent of extra pure grade; used without further purification.

**Estimated Error:**
Temperature: control to ±0.005 K.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]

**Original Measurements:**
J. R. Battler and R. L. Rowley, J. Chem. Eng. Data **35**, 334–8 (1990).

**Variables:**
$T$/K = 293 and 302

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of nitroethane (1) in 2,2,4-trimethylpentane (2) at 293 K was reported to be $x_1 = 0.20$. The corresponding mass percentage calculated by the compiler is $100\ w_1 = 14.1$.

The solubility of 2,2,4-trimethylpentane (2) in nitroethane (1) at 293 K was reported to be $x_2 = 0.17$. The corresponding mass percentage calculated by the compiler is $100\ w_2 = 23.8$.

The upper critical solution temperature was reported to be 302.15 K.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; spectrophotometric grade; 99.9 mole % purity.
(2) Source not specified; spectrophotometric grade; 99.9 mole % purity.

**Estimated Error:**
Not specified.

## 3.16. Octane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Octane; $C_8H_{18}$ ; [111-65-9]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 273–314

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Mutual solubility of nitroethane (1) and octane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $100\ w_1$ | $x_1$ (compilers) | $100\ w_1$ | $x_1$ (compilers) |
| 0.0 | 273.15 | 5.8 | 0.086 | 91.0 | 0.939 |
| 4.20 | 277.35 | 5.9 | 0.087 | 90.8 | 0.938 |
| 6.50 | 279.65 | 6.5 | 0.096 | 90.3 | 0.934 |
| 10.70 | 283.85 | 7.6 | 0.111 | 89.3 | 0.927 |
| 14.2[a] | 287.35 | 8.57 | 0.125 | ··· | ··· |
| 14.85 | 288.00 | 9.0 | 0.131 | 87.7 | 0.916 |
| 16.85 | 290.00 | 9.9 | 0.143 | 86.8 | 0.909 |
| 18.40 | 291.55 | 10.5 | 0.151 | 86.3 | 0.906 |
| 20.80 | 293.95 | 11.5 | 0.165 | 85.0 | 0.896 |
| 21.60[a] | 294.15 | ··· | ··· | 85.0 | 0.896 |
| 23.3[a] | 296.45 | 12.3 | 0.176 | ··· | ··· |
| 26.0[a] | 299.15 | ··· | ··· | 82.35 | 0.877 |
| 28.3[a] | 301.45 | 15.49 | 0.218 | ··· | ··· |
| 32.8[a] | 305.95 | ··· | ··· | 76.86 | 0.835 |
| 34.6[a] | 307.75 | 21.37 | 0.293 | ··· | ··· |
| 39.5[a] | 312.65 | 30.88 | 0.405 | ··· | ··· |
| 39.6[a] | 312.75 | ··· | ··· | 65.08 | 0.739 |
| 41.3[a] | 314.45 | 49.01 | 0.594 | ··· | ··· |
| 41.3 | 314.45 | ··· | ··· | ··· | ··· (UCST) |

[a]Obtained by synthetic method. All other data obtained by the analytical method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to 0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**
[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

## 3.17. Nonanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Nonanoic acid; $C_9H_{18}O_2$; [112-05-0]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273 and 283

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Solubility of nonanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 45.0 | 31.0 | 0.176 |
| 10.0 | 283.2 | 2340 | 95.9 | 0.917 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*,[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*[1] (dried and twice distilled).
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point = 12.25 °C.

**Estimated Error:**
Not reported.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.18. Nonane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Nonane; $C_9H_{20}$; [111-84-2]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 290–323

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and nonane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1$ | $100\,w_1$ (compilers) | $x_1$ | $100\,w_1$ (compilers) |
| 16.3 | 289.5 | ··· | ··· | 0.940 | 90.2 |
| 37.9 | 311.1 | ··· | ··· | 0.875 | 80.4 |
| 42.4 | 315.6 | 0.315 | 21.2 | ··· | ··· |
| 45.8 | 319.0 | ··· | ··· | 0.810 | 71.4 |
| 48.9 | 322.1 | 0.460 | 33.3 | ··· | ··· |
| 49.1 | 322.3 | ··· | ··· | 0.715 | 59.5 |
| 49.5 | 322.7 | ··· | ··· | 0.605 | 47.3 |
| 49.5 | 322.7 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solutions of (1) and (2) were prepared by weight from glass syringes in 13 mm×100 mm Kimax screw cap culture tubes and sealed by a cap with a Teflon faced rubber liner. The tubes were suspended in a 3 L well-stirred water bath and cloud points observed visually. At least two observations were made of each set of samples: the first at a relatively fast cooling rate to find the approximate cloud point temperature and the second at a slow cooling rate to more precisely determine the cloud point temperature.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled at 57 °C/12.9 kPa.
(2) Phillips; purity 99 mole %.

**Estimated Error:**
Temperature: control to ±0.1 K.

## 3.19. 1-Nonanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

### Critical Evaluation

Solubilities in the system nitroethane (1)+1-nonanol (2) were reported in two publications. Zhuravleva *et al.*[1] carried out measurement of the mutual solubilities of the two components between 252 and 284 K by the synthetic method. Zhuravleva and Zhukova[2] determined the mutual solubility of two components by the synthetic method between 266 and 290 K.

The upper critical solution temperature has been reported as 284.2 K (Zhuravleva *et al.*[1]) and 289.7 K;[2] the difference is very large and is equal to 5.5 K. Both results have been measured by the same main investigator. In the opinion of the evaluator the value 289.7 K (Zhuravleva and Zhukova[2]) should be treated as tentative because it was published 1 yr later. It may be treated as the improved value and this value is in agreement with other UCST of the nitroethane–alcohol systems published in this collection. Therefore the UCST reported in Zhuravleva *et al.*[1] is rejected as well as other data from the Zhuravleva *et al.*[1] Thus the tentative values of the critical point are those reported in Zhuravleva and Zhukova:[2] $T_c = 289.7$ K and $x_{c1} = 0.684$. They were used in the approximation of solubility data. Monotectic equilibrium is realized at 265.9 K.[2]

The experimental data reported in Zhuravleva and Zhukova[2] have been approximated (with the same weighing factor) by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1 = 0.83415,\ a_2 = 0.11334,\ b_1 = 5.72965,\ b_2 = -5.17458\ \text{(mean standard error of estimate was 0.0097)}.$$

For this approximation values of $x_{c1} = 0.684$ and $T_c = 289.7$ have been used. In the opinion of the evaluator, all experimental solubility data and the smoothed mutual solubility, calculated by this equation, may be treated as tentative. The results of calculations for selected temperatures are presented in the following table. This relationship together with experimental points (Zhuravleva and Zhukova[2]) are also presented in Fig. 8.

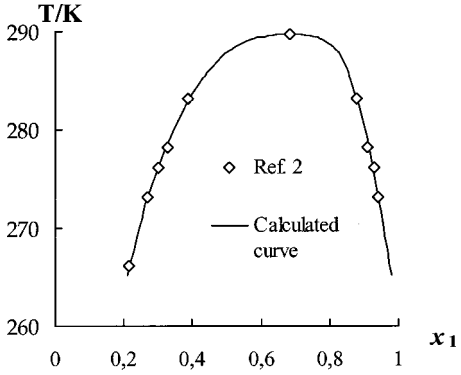


FIG. 8. Mutual solubility of nitroethane and 1-nonanol.

Mutual solubility of nitroethane and 1-nonanol

| | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|
| $T$/K | $x_1$ | 100 $w_1$ | $x_1$ | 100 $w_1$ |
| 270.2 | 0.246 | 14.5 | 0.956 | 91.9 |
| 273.2 | 0.271 | 16.2 | 0.942 | 89.4 |
| 276.2 | 0.300 | 18.2 | 0.926 | 86.7 |
| 279.2 | 0.334 | 20.7 | 0.909 | 83.9 |
| 283.2 | 0.392 | 25.1 | 0.880 | 79.2 |
| 285.2 | 0.430 | 28.2 | 0.861 | 76.3 |
| 287.2 | 0.481 | 32.5 | 0.835 | 72.5 |
| 288.2 | 0.517 | 35.8 | 0.815 | 69.6 |
| 289.2 | 0.572 | 41.0 | 0.779 | 64.7 |
| 289.4 | 0.591 | 42.9 | 0.766 | 63.0 |
| 289.6 | 0.621 | 46.0 | 0.742 | 59.9 |

**References:**

[1]I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976); Deposited Doc., VINITI 1951 (1976).

[2]I. K. Zhuravleva and L. M. Zhukova, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **20**, 516 (1977).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

**Original Measurements:**
I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976).
*Deposited Doc., VINITI 1951 (1976).

**Variables:**
$T$/K = 252–284

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-nonanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| −21.0 | 252.2 | 10.0 | 0.176 | ··· | ··· |
| 0.0 | 273.2 | 20.0 | 0.325 | 90.0 | 0.945 |
| 5.5 | 278.7 | ··· | ··· | 80.0 | 0.885 |
| 7.0 | 280.2 | 30.0 | 0.452 | ··· | ··· |
| 9.5 | 282.7 | ··· | ··· | 70.0 | 0.818 |
| 10.0 | 283.2 | 40.0 | 0.562 | ··· | ··· |
| 10.5 | 283.7 | 50.0 | 0.678 | 60.0 | 0.742 |
| 11.0 | 284.2 | 55.5 | 0.705 | 55.5 | 0.705 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method (Alekseev[1]) was used.
No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; $n$(20 °C,D) = 1.3905, $d$(20 °C,4 °C) = 1.0525.
(2) Source not specified; purity not specified; $n$(20 °C,D) = 1.4300, $d$(20 °C,4 °C) = 0.8270.

**Estimated Error:**
Not specified.

**References:**
[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

**Original Measurements:**
I. K. Zhuravleva and L. M. Zhukova, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **20**, 516–8 (1977).

**Variables:**
$T$/K = 266–290

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-nonanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1$ | $x_1$ (compiler) | 100 $w_1$ | $x_1$ (compiler) |
| −7.0 | 266.2 | 12.5 | 0.215 | ··· | ··· |
| 0.0 | 273.2 | 16.2 | 0.271 | 89.3 | 0.941 |
| 3.0 | 276.2 | 18.2 | 0.300 | 87.3 | 0.930 |
| 5.0 | 278.2 | 20.2 | 0.327 | 84.4 | 0.912 |
| 10.0 | 283.2 | 24.8 | 0.388 | 79.2 | 0.880 |
| 16.5 | 289.7 | 53.0 | 0.684 | 53.0 | 0.684 (UCST) |

Monotectic equilibrium occurs at 265.9 K.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; distilled; boiling point = 114 °C; $n$(20 °C,D) = 1.3910, $d$(20 °C,4 °C) = 1.052.
(2) Source not specified; distilled; boiling point = 213 °C; melting point = 5.3 °C; $n$(20 °C,D) = 1.4310, $d$(20 °C,4 °C) = 0.828.

**Estimated Error:**
Not specified.

## 3.20. Decanenitrile

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Decanenitrile; $C_{10}H_{19}N$; [1975-78-6]

**Original Measurements:**
C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68–80 (1944).

**Variables:**
$T$/K = 233–255

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of decanenitrile (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of decanenitrile (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −40.0 | 233.2 | 23.6 | 19.1 | 0.104 |
| −39.9* | 233.3 | ··· | 20.0 | 0.109 |
| −34.5* | 238.7 | ··· | 24.7 | 0.138 |
| −30.0* | 243.2 | ··· | 38.6 | 0.235 |
| −27.7* | 245.5 | ··· | 48.2 | 0.313 |
| −23.4* | 249.8 | ··· | 67.5 | 0.505 |
| −20.0 | 253.2 | 455 | 82.0 | 0.691 |
| −18.5* | 254.7 | ··· | 88.5 | 0.790 |

*These data were extracted by the compilers from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron-constantan thermocouple. As the nitrile crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing the decanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Stedman packed column; freezing point = −14.46 °C.

**Estimated Error:**
Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

## 3.21. Decanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Decanoic acid; $C_{10}H_{20}O_2$; [334-48-5]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273–303

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility of decanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 9.2 | 8.4 | 0.039 |
| 10.0 | 283.2 | 12.5 | 11.1 | 0.052 |
| 20.0 | 293.2 | 55.0 | 35.5 | 0.193 |
| 30.0 | 303.2 | 7000 | 98.6 | 0.968 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*,[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*[1] (dried and twice distilled).
(2) Purified according to Pool and Ralston;[2] freezing point = 31.24 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.22. Decanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Decanamide; $C_{10}H_{21}NO$; [2319-29-1]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K=283–365

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of decanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of decanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.8 | 0.8 | 0.004 |
| 30.0 | 303.2 | 1.1 | 1.1 | 0.005 |
| 38.5* | 311.7 | ··· | 2.0 | 0.009 |
| 45.5* | 318.7 | ··· | 2.9 | 0.013 |
| 50.0 | 323.2 | 4.2 | 4.0 | 0.018 |
| 59.1* | 332.3 | ··· | 7.6 | 0.035 |
| 62.5* | 335.7 | ··· | 10.1 | 0.047 |
| 70.0 | 343.2 | 25.2 | 20.1 | 0.100 |
| 70.7* | 343.9 | ··· | 20.9 | 0.104 |
| 76.2* | 349.4 | ··· | 38.3 | 0.214 |
| 81.7* | 354.9 | ··· | 60.0 | 0.397 |
| 87.9* | 361.1 | ··· | 84.0 | 0.697 |
| 90.0 | 363.2 | 850 | 89.5 | 0.788 |
| 91.9* | 365.1 | ··· | 92.6 | 0.846 |

*These data were extracted by the compilers from the published graphs.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the octanoic acid at 190–210 °C for 10–14 h; purified by recrystallization; freezing point=98.5 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.23. Decane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

### Critical Evaluation

Solubilities in the system nitroethane (1)+decane (2) were reported in three publications. Francis[1] determined the upper critical solution temperature (UCST). Hwa *et al.*[2] measured of the mutual solubilities of the two components between 275 and 326 K by the synthetic and analytical methods. Clever *et al.*[3] determined solubility of nitroethane in decane at 331.2 K by the synthetic method.

The upper critical solution temperature has been reported as 323.2 K (Francis[1]) and 325.8 K (Hwa *et al.*[2]). The critical solution concentration is determined as $x_{c1}=0.63\pm0.01$ by the evaluator on the basis of the solubility curve of binary system.[2]

The experimental data reported in Hwa *et al.*[2] have been approximated (with the same weighing factor) by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1=0.797\,47,\ a_2=0.159\,37,\ b_1=1.228\,59,\ b_2=-1.559\,33\ \text{(mean standard error of estimate was 0.0430)}.$$

For this approximation values $x_{c1}$ and UCST from Hwa *et al.*[2] were used. In the opinion of the evaluator, all experimental solubility data and the smoothed mutual solubility, calculated by this equation, may be treated as tentative. The results of calculations for selected temperatures are presented in the table below. This relationship together with experimental points[2] are also presented in Fig. 9.

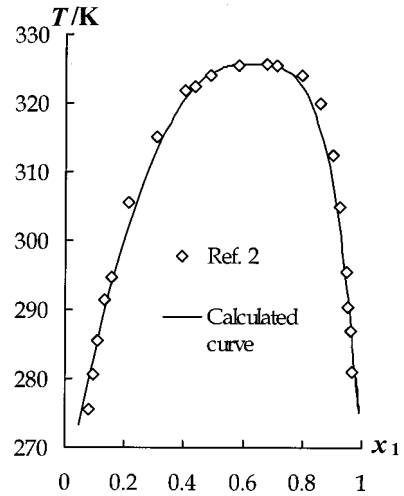


FIG. 9. Mutual solubility of nitroethane and decane.

Mutual solubility of nitroethane and decane

| | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|
| $T$/K | $x_1$ | 100 $w_1$ | $x_1$ | 100 $w_1$ |
| 278.2 | 0.072 | 3.9 | 0.984 | 97.0 |
| 283.2 | 0.098 | 5.4 | 0.973 | 95.0 |
| 288.2 | 0.125 | 7.0 | 0.962 | 93.0 |
| 293.2 | 0.154 | 8.8 | 0.950 | 90.9 |
| 298.2 | 0.186 | 10.7 | 0.935 | 88.4 |
| 303.2 | 0.221 | 13.0 | 0.919 | 85.7 |
| 308.2 | 0.261 | 15.7 | 0.900 | 82.6 |
| 313.2 | 0.307 | 18.9 | 0.876 | 78.8 |
| 318.2 | 0.365 | 23.3 | 0.842 | 73.8 |
| 319.2 | 0.379 | 24.3 | 0.834 | 72.6 |
| 320.2 | 0.394 | 25.5 | 0.824 | 71.2 |
| 321.2 | 0.411 | 26.9 | 0.813 | 69.6 |
| 322.2 | 0.430 | 28.5 | 0.800 | 67.8 |
| 323.2 | 0.453 | 30.4 | 0.784 | 65.7 |
| 324.2 | 0.482 | 32.9 | 0.763 | 62.9 |
| 325.2 | 0.525 | 36.8 | 0.728 | 58.5 |

**References:**

[1]A. W. Francis, ''Critical Solution Temperature,'' Adv. Chem. Ser. **31** (1961).
[2]S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409 (1963).
[3]H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31 (1972).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K = 275–326

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Mutual solubility of nitroethane (1) and decane (2)

| | | Decane-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 2.33[a] | 275.48 | 4.4 | 0.080 | ··· | ··· |
| 7.40[a] | 280.55 | 5.2 | 0.094 | ··· | ··· |
| 7.80[a] | 280.95 | ··· | ··· | 94.3 | 0.969 |
| 12.45[a] | 285.60 | 6.2 | 0.111 | ··· | ··· |
| 13.80[a] | 286.95 | ··· | ··· | 92.8 | 0.961 |
| 17.20[a] | 290.35 | ··· | ··· | 91.6 | 0.954 |
| 18.20[a] | 291.35 | 7.6 | 0.135 | ··· | ··· |
| 21.50[a] | 294.65 | 8.8 | 0.155 | ··· | ··· |
| 22.40[a] | 295.55 | ··· | ··· | 90.4 | 0.947 |
| 31.8[b] | 305.0 | ··· | ··· | 86.8 | 0.926 |
| 32.4[b] | 305.6 | 12.65 | 0.215 | ··· | ··· |
| 39.3[b] | 312.5 | ··· | ··· | 82.62 | 0.900 |
| 42.0[b] | 315.2 | 19.05 | 0.308 | ··· | ··· |
| 46.8[b] | 320.0 | ··· | ··· | 76.13 | 0.858 |
| 48.6[b] | 321.8 | 26.20 | 0.402 | ··· | ··· |
| 49.3[b] | 322.5 | 28.96 | 0.436 | ··· | ··· |
| 50.8[b] | 324.0 | 33.30 | 0.486 | 67.54 | 0.798 |
| 52.3[b] | 325.5 | 42.22 | 0.581 | ··· | ··· |
| 52.4[b] | 325.6 | ··· | ··· | 56.20 | 0.709 |
| 52.6[b] | 325.8 | ··· | ··· | 52.47 | 0.677 |
| 52.6 | 325.8 | ··· | ··· | ··· | ··· (UCST) |

[a]Only one of the equilibrium phases was analyzed at each temperature.
[b]Obtained by synthetic method.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic and analytical methods were used as described in Vold and Vold.[1] The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques. The temperature of the bath was controlled to ±0.05 K.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: to 0.1 K (synthetic method);
Composition: ±0.5 mass % (analytical method).

**References:**

[1]R. D. Vold and M. J. Vold, *Physical Methods of Organic Chemistry*, Vol. 1 (Interscience, New York, 1945).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Decane; $C_{10}H_{22}$ ; [124-18-5]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K=331

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Solubility of nitroethane (1) in decane (2) at 58.0 °C (331.2 K) was reported to be $x_1=0.730$ (100 $w_1=58.8$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solutions of (1) and (2) were prepared by mass from glass syringes in 13 mm×100 mm Kimax screw cap culture tubes and sealed with a Teflon-faced rubber liner. Tubes were immersed in a 3 L stirred water bath. Two cloud point observations were made visually: one at a relatively fast cooling rate, and the second at a slow cooling rate to more precisely determine cloud point temperature.

**Source and Purity of Materials:**
(1) Matheson, Coleman and Bell; practical grade; distilled at 57 °C/12.9 kPa.
(2) Phillips; purity 99 mol %.

**Estimated Error:**
Temperature: ±0.1 K.

## 3.24. 1-Decanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for nitroethane (1)+1-decanol (2) have been reported in the four publications listed in Table 1.

Table 1. Summary of solubility data for the system nitroethane +1-decanol

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Hoerr *et al.*[1] | 256–293 | mutual | synthetic |
| Francis[2] | 273–292 | mutual | synthetic |
| Zhuravleva *et al.*[3] | 277–294 | mutual | synthetic |
| Majgler-Baranowska *et al.*[4] | 288–294 | mutual | synthetic |

The original data are compiled immediately following this Critical Evaluation. The data of Francis[2] (nitroethane-rich phase only) are in marked disagreement with other studies and have been rejected. All other reported data are used in Table 2.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in Table 2. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of nitroethane and 1-decanol

| | Alcohol-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|
| $T$/K | 100 $w_1$ | $x_1$ | | 100 $w_2$ | $x_2$ | |
| 273.2 | ··· | ··· | ··· | 6.6 | 0.032 | tentative |
| 278.2 | 17 | 0.30 | tentative | 10.8 | 0.054 | recommended |
| 283.2 | 20 | 0.34 | tentative | 15.0 | 0.077 | recommended |
| 288.2 | 25.4 | 0.418 | tentative | 18.5 | 0.097 | tentative |
| 293.2 | 39.0 | 0.574 | tentative | 30.0 | 0.169 | tentative |

The upper critical solution temperature (UCST) has been reported as 291.6 K,[2] 294.2 K,[3] and 294.4 K.[4] The UCST of Francis[2] is rejected. Thus, the recommended value are: $T_c$=294.3±0.1 K.

The corresponding critical solution composition has been reported as $x_{c1}=0.704$,[2] $x_{c1}=0.713$,[4] $x_{c1}=0.716$.[3] The mean value $x_{c1}=0.711\pm0.005$, is recommended.

The recommended and tentative values for the mutual solubility reported in Table 2 have been approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived: $a_1=0.755\,04$, $a_2=0.589\,94$, $b_1=2.756\,47$, $b_2=-3.411\,96$ (mean standard error of estimate was 0.0176).

For this approximation, the recommended values of UCST and $x_{c1}$ were used. This relationship is presented in Fig. 10 together with experimental data reported in the four references.[1–4]

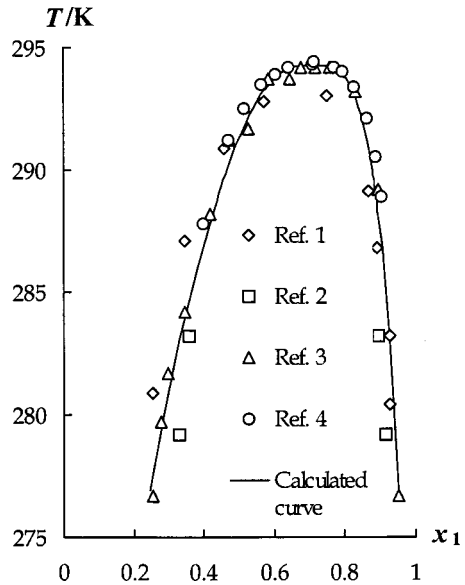


FIG. 10. Mutual solubility of nitroethane and 1-decanol.

**References:**

[1]C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267 (1944).

[2]A. W. Francis, J. Phys. Chem. **60**, 20 (1956).

[3]I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976); Deposited Doc., VINITI 1951 (1976).

[4]H. Majgler-Baranowska, W. Pyzuk, W. Jeute, and J. Ziolo, J. Chem. Eng. Data **26**, 51 (1981).

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Original Measurements:**

C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267–80 (1944).

**Variables:**

$T$/K = 256–293

**Prepared By:**

N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of nitroethane (1) and 1-decanol (2) in mass percent including the region of immiscible solution over the temperature range were presented in graphical form and in a table.

Mutual solubility of nitroethane (1) and 1-decanol (2)

| | | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| −17.3* | 255.9 | ··· | ··· | ··· | 99.0[a] | 0.995 |
| −10.0* | 263.2 | ··· | ··· | ··· | 98.5[a] | 0.993 |
| −4.5* | 268.7 | ··· | ··· | ··· | 97.0[a] | 0.985 |
| 0.0 | 273.2 | 7.1 | ··· | ··· | 93.4[a] | 0.968 |
| 2.7* | 275.9 | ··· | ··· | ··· | 89.3[a] | 0.946 |
| 3.8* | 277.0 | ··· | 8.2[a] | 0.158 | ··· | ··· |
| 5.1* | 278.3 | ··· | 3.7[a] | 0.075 | ··· | ··· |
| 7.2* | 280.4 | ··· | ··· | ··· | 86.2[b] | 0.929 |
| 7.7* | 280.9 | ··· | 13.9[b] | 0.254 | ··· | ··· |
| 10.0 | 283.2 | 16.9 | ··· | ··· | 85.5[b] | 0.926 |
| 13.6* | 286.8 | ··· | ··· | ··· | 79.7[b] | 0.892 |
| 13.9* | 287.1 | ··· | 20.0[b] | 0.345 | ··· | ··· |
| 15.9* | 289.1 | ··· | ··· | ··· | 75.5[b] | 0.867 |
| 17.7* | 290.9 | ··· | 28.9[b] | 0.461 | ··· | ··· |
| 19.6* | 292.8 | ··· | 38.8[b] | 0.572 | ··· | ··· |
| 19.8* | 293.0 | ··· | ··· | ··· | 59.0[b] | 0.752 |

*Data extracted from the published graphs by the compilers.
[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium occurs at 276.6 K.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The solubility measurements were made with the equipment and in the manner described in Hoerr *et al.*[1] and Ralston *et al.*[2]

**Source and Purity of Materials:**

(1) Source not specified; purity not specified.
(2) Prepared by catalytic hydrogenation of ethyl caprate; purified by vacuum distillation; freezing point = 6.88 °C.

**Estimated Error:**

Not specified.

**References:**

[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).

[2]A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. **9**, 102 (1944).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Original Measurements:**
A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

**Variables:**
$T$/K = 273–292

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-decanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 0.0 | 273.2 | ··· | ··· | 90.0 | 0.950 |
| 6.0 | 279.2 | 19.0 | 0.331 | 84.0 | 0.917 |
| 10.0 | 283.2 | 21.0 | 0.359 | 80.0 | 0.894 |
| 18.4 | 291.6 | 53.0 | 0.704 | 53.0 | 0.704 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The observations were made after vigorously shaking on glass stoppered graduated tubes of about 15 mL capacity immersed in water baths in large Dewar flasks. The water was agitated with a rapid stream of air bubbles. The temperature was adjusted by adding small amounts of cooler or warmer water occasionally as required.

**Source and Purity of Materials:**
(1) Eastman Kodak Co.; distilled with 30 cm column with reflux; boiling point = 114–115 °C; $n$(20 °C,D) = 1.3920, $\rho$(20 °C) = 1046.9 g·L$^{-1}$.
(2) Source not specified; purified by crystallization; melting point = 6.8 °C; $n$(20 °C,D) = 1.4372, $\rho$(20 °C) = 831.8 g·L$^{-1}$.

**Estimated Error:**
Not specified.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Original Measurements:**
I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976).
*Deposited Doc., VINITI 1951 (1976).

**Variables:**
$T$/K = 277–294

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-decanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 3.5 | 276.7 | 14.0 | 0.255 | 90.0 | 0.950 |
| 6.5 | 279.7 | 15.5 | 0.279 | ··· | ··· |
| 8.5 | 281.7 | 16.8 | 0.299 | ··· | ··· |
| 11.0 | 284.2 | 20.0 | 0.345 | ··· | ··· |
| 15.0 | 288.2 | 25.4 | 0.418 | ··· | ··· |
| 16.0 | 289.2 | ··· | ··· | 80.0 | 0.894 |
| 18.0 | 291.2 | 30.0 | 0.475 | ··· | ··· |
| 18.5 | 291.7 | 34.7 | 0.528 | ··· | ··· |
| 20.0 | 293.2 | ··· | ··· | 70.0 | 0.831 |
| 20.5 | 293.7 | 40.0 | 0.584 | ··· | ··· |
| 20.5 | 293.7 | 46.5 | 0.647 | ··· | ··· |
| 21.0 | 294.2 | 50.0 | 0.678 | 60.0 | 0.760 |
| 21.0 | 294.2 | 54.5 | 0.716 | 54.5 | 0.716 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method (Alekseev[1]) was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; $n$(20 °C,D) = 1.3905, $d$(20 °C,4 °C) = 1.0525.
(2) Source not specified; purity not specified; $n$(25 °C,D) = 1.4370, $d$(20 °C,4 °C) = 0.830.

**Estimated Error:**
Not specified.

**References:**
[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Original Measurements:**
H. Majgler-Baranowska, W. Pyzuk, W. Jeute, and J. Ziolo, J. Chem. Eng. Data **26**, 51–3 (1981).

**Variables:**
$T$/K = 288–294

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual solubility of nitroethane (1) and 1-decanol (2) in volume fractions is presented over the temperature range in graphical form.

Mutual solubility of nitroethane (1) and 1-decanol (2)

| | | Alcohol-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|---|
| $T$/K | $t$/°C (compilers) | $\varnothing_1$ | 100 $w_1$ (compilers) | $x_1$ (compilers) | $\varnothing_1$ | 100 $w_1$ (compilers) | $x_1$ (compilers) |
| 287.8 | 14.6 | 0.200 | 24.1 | 0.401 | ··· | ··· | ··· |
| 288.9 | 15.7 | ··· | ··· | ··· | 0.774 | 81.3 | 0.902 |
| 290.5 | 17.3 | ··· | ··· | ··· | 0.745 | 78.8 | 0.887 |
| 291.2 | 18.0 | 0.249 | 29.6 | 0.470 | ··· | ··· | ··· |
| 292.1 | 18.9 | ··· | ··· | ··· | 0.700 | 74.8 | 0.862 |
| 292.5 | 19.3 | 0.286 | 33.7 | 0.517 | ··· | ··· | ··· |
| 293.4 | 20.2 | ··· | ··· | ··· | 0.640 | 69.3 | 0.826 |
| 293.5 | 20.3 | 0.326 | 38.0 | 0.564 | ··· | ··· | ··· |
| 293.9 | 20.7 | 0.362 | 41.9 | 0.603 | ··· | ··· | ··· |
| 294.0 | 20.8 | ··· | ··· | ··· | 0.592 | 64.8 | 0.795 |
| 294.2 | 21.0 | 0.400 | 45.8 | 0.641 | 0.557 | 61.5 | 0.771 |
| 294.3 | 21.1 | 0.477 | 53.7 | 0.709 | ··· | ··· | ··· |
| 294.4 | 21.2 | 0.483 | 54.3 | 0.715 | 0.483 | 54.3 | 0.715 (UCST) |

Data extracted from the published graphs by the compilers. For conversions of volume concentration utilized values of density of nitroethane $\rho$(20 °C)=1052.8 g·L$^{-1}$, Weissberger *et al.*[1] and 1-decanol $\rho$(20 °C)=829.2 g·L$^{-1}$, Marsdne and Mann,[2] at 293.2 K (20.0 °C).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Miscibility temperature was determined by observing turbidity changes during heating and cooling of vigorously shaken solutions. No experimental details given.

**Source and Purity of Materials:**
(1) Fluka; initial purity 95 mass %; purified agitation with sulfuric acid, washing, dried and distilled under reduced pressure over $CaSO_4$.
(2) Source not specified; purity 98 mass %; dried, vacuum fractionated and redistilled over $CaH_2$.

**Estimated Error:**
Temperature: ±0.05 K.

**References:**
[1]A. Weissberger, E. S. Proskauer, J. A. Riddick, and E. E. Toops, Jr., *Organic Solvents* (Interscience, New York, 1955).
[2]C. Marsden and S. Mann, *Solvents Guide* (Cleaver-Hume, London, 1963).

## 3.25. Undecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Undecanoic acid; $C_{11}H_{22}O_2$; [112-37-8]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273–293

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Solubility of undecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 8.1 | 7.5 | 0.032 |
| 10.0 | 283.2 | 13.2 | 11.7 | 0.051 |
| 20.0 | 293.2 | 131.0 | 56.7 | 0.345 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*[1] (dried and twice distilled).
(2) Purified according to Pool and Ralston,[2] freezing point = 28.13 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.26. Heptacosafluorotributanamine

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Heptacosafluorotributanamine; $C_{12}H_{27}N$; [311-89-7]

**Original Measurements:**
J. Vreeland and R. Dunlap, J. Phys. Chem. **61**, 329–33 (1957).

**Variables:**
$T$/K = 298

**Prepared By:**
V. P. Sazonov and N. I. Lisov

### Experimental Data

The solubility of nitroethane (1) in heptacosafluorotributanamine (2) at 298 K was reported to be 100 $w_1$ = 0.1. The corresponding mole fraction, $x_1$ , calculated by the compilers is 0.009.

The solubility of heptacosafluorotributanamine (2) in nitroethane (1) at 298 K was reported to be 100 $w_2$ = 0.1. The corresponding mole fraction $x_2$ calculated by the compiler is 0.0001.

### Auxiliary Information

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Matheson Chemical Co.; research grade; distilled through a Todd column; boiling point = 114.7 °C–114.8 °C.
(2) Minnesota Mining and Manufacturing Co.; distilled; boiling point = 178.8 °C–179.1 °C.

**Estimated Error:**
Not specified.

## 3.27. Dodecanenitrile

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Dodecanenitrile; $C_{12}H_{23}N$; [2437-25-4]

**Original Measurements:**
C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68–80 (1944).

**Variables:**
$T$/K = 233–273

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of dodecanenitrile (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of dodecanenitrile (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −40.0 | 233.2 | 7.9 | 7.3 | 0.032 |
| −38.0* | 235.2 | ··· | 7.7 | 0.033 |
| −30.9* | 242.3 | ··· | 10.0 | 0.044 |
| −22.1* | 251.1 | ··· | 15.7 | 0.071 |
| −20.0 | 253.2 | 22.1 | 18.1 | 0.084 |
| −18.5* | 254.7 | ··· | 20.4 | 0.096 |
| −14.5* | 258.7 | ··· | 30.5 | 0.153 |
| −10.8* | 262.4 | ··· | 46.5 | 0.264 |
| −7.0* | 266.2 | ··· | 62.5 | 0.407 |
| −4.4* | 268.8 | ··· | 74.0 | 0.540 |
| −1.2* | 272.0 | ··· | 85.5 | 0.708 |
| 0.0 | 273.2 | 830 | 89.2 | 0.774 |

*Data extracted from the published graphs by the compilers.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron-constantan thermocouple. As the nitrile crystallized from the solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing the dodecanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Stedman packed column; freezing point = 4.02 °C.

**Estimated Error:**
Temperature ±0.4 K (below 248 K), ±0.2 K (above 248 K).

## 3.28. Dodecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Dodecanoic acid; $C_{12}H_{24}O_2$; [143-07-7]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273–313

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Solubility of dodecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 1.9 | 1.8 | 0.007 |
| 10.0 | 283.2 | 2.8 | 2.7 | 0.010 |
| 20.0 | 293.2 | 5.4 | 5.1 | 0.020 |
| 30.0 | 303.2 | 16.3 | 14.0 | 0.058 |
| 40.0 | 313.2 | 1460 | 93.6 | 0.846 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*[1] (dried and twice distilled).
(2) Source not specified; purified according to Pool and Ralston,[2] freezing point=43.92 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.29. Dodecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Dodecanamide; $C_{12}H_{25}NO$; [1120-16-7]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–373

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**
The solubilities of dodecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of dodecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.8 | 0.8 | 0.003 |
| 30.0 | 303.2 | 1.1 | 1.1 | 0.004 |
| 45.5* | 318.7 | ··· | 2.9 | 0.011 |
| 50.0 | 323.2 | 3.9 | 3.8 | 0.015 |
| 64.4* | 337.6 | ··· | 10.9 | 0.044 |
| 70.0 | 343.2 | 24.2 | 19.5 | 0.084 |
| 70.9* | 344.1 | ··· | 21.1 | 0.092 |
| 74.1* | 347.3 | ··· | 28.2 | 0.129 |
| 77.6* | 350.8 | ··· | 39.4 | 0.197 |
| 82.9* | 356.1 | ··· | 58.5 | 0.347 |
| 89.4* | 362.6 | ··· | 80.9 | 0.615 |
| 90.0 | 363.2 | 495 | 83.2 | 0.651 |
| 93.9* | 367.1 | ··· | 90.9 | 0.790 |
| 100.0 | 373.2 | 5100 | 98.1 | 0.951 |

*Data extracted from the published graphs by the compilers.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the dodecanoic acid at 190–210 °C for 10–14 h; purified by recrystallization; freezing point=102.4 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.30. 1-Dodecanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system nitroethane (1) +1-dodecanol (2) were reported in the publications listed in Table 1.

Table 1. Summary of solubility data for the system nitroethane +1-dodecanol

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Hoerr *et al.*[1] | 268–302 | mutual | synthetic |
| Francis[2] | 287–300 | mutual | synthetic |
| Zhuravlev and Erofeeva[3] | 294–302 | mutual | synthetic |

The original data are compiled immediately following this Critical Evaluation. All reported data are used in Table 2 below.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in Table 2. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of nitroethane (1) and 1-dodecanol (2)

| | Alcohol-rich phase | | | Nitroethane-rich phase | | |
|---|---|---|---|---|---|---|
| $T$/K | 100 $w_1$ | $x_1$ | | 100 $w_2$ | $x_2$ | |
| 293.2 | 23.0 | 0.426 | tentative | 16.4 | 0.074 | recommended |
| 295.2 | 25.3 | 0.457 | recommended | 19.8 | 0.090 | recommended |
| 297.2 | 29.0 | 0.503 | recommended | 24.0 | 0.113 | recommended |
| 299.2 | 31.5 | 0.533 | tentative | 28.0 | 0.135 | tentative |
| 301.2 | 42.5 | 0.647 | tentative | 39.5 | 0.208 | tentative |

The upper critical solution temperature has been reported as 299.7 K (Francis[2]) and 301.6 K;[3] the difference is equal to 1.9 K. In the opinion of the evaluator the value 301.6 K (Zhuravlev and Erofeeva[3]) should be treated as tentative because this value is in the agreement with other UCST of the nitroethane–alcohol systems published in this collection. Therefore the UCST reported in Francis[2] is rejected, the same as UCST for other systems of the series reported in this paper. Thus the tentative values of the critical point are those reported in Zhuravlev and Erofeeva:[3] $T_c$=301.6 K and $x_{c1}$=0.733. They were used in the approximation of solubility data.

The recommended and tentative values for the mutual solubility reported in the above table were approximated by an equation based on the scaling law (described in the preface to this volume) for which the following parameters were derived:

$$a_1=0.739\ 71,\ a_2=0.363\ 64,\ b_1=8.929\ 22,\ b_2=-7.362\ 71 \quad \text{(mean standard error of estimate was 0.0044).}$$

For this approximation, the values of UCST and $x_{c1}$ were used from Zhuravlev and Erofeeva.[3] This relationship is presented in Fig. 11 together with experimental data reported in the three references.[1–3]

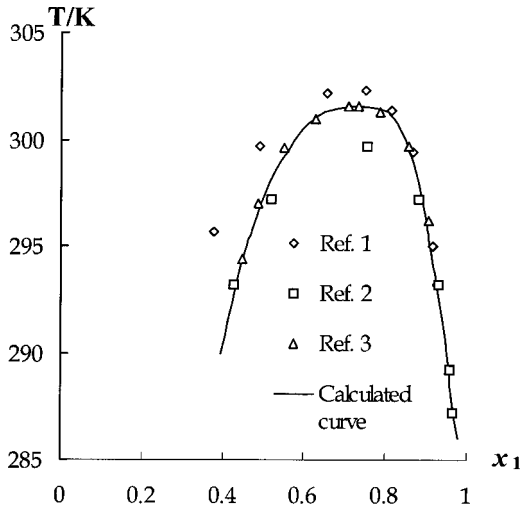


FIG. 11. Mutual solubility of nitroethane and 1-dodecanol.

**References:**
[1]C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267 (1944).
[2]A. W. Francis, J. Phys. Chem. **60**, 20 (1956).
[3]E. F. Zhuravlev and F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10 (1968).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**
C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267–80 (1944).

**Variables:**
$T$/K = 268–302

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of nitroethane (1) and 1-dodecanol (2) in mass percent including the region of immiscible solution over the temperature range were presented in graphical form and in a table.

Mutual solubility of nitroethane (1) and 1-dodecanol (2)

| | | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| −5.5* | 267.7 | ··· | ··· | ··· | 99.7[a] | 0.000 |
| 0.0 | 273.2 | 0.9 | ··· | ··· | 99.1[a] | 0.996 |
| 1.1* | 274.3 | ··· | ··· | ··· | 99.0[a] | 0.995 |
| 8.0* | 281.2 | ··· | ··· | ··· | 97.0[a] | 0.988 |
| 10.0 | 283.2 | 4.2 | ··· | ··· | 96.0[a] | 0.983 |
| 13.5* | 284.7 | ··· | ··· | ··· | 93.6[a] | 0.973 |
| 18.6* | 291.8 | ··· | ··· | ··· | 87.0[a] | 0.943 |
| 19.3* | 292.5 | ··· | 12.2[a] | 0.256 | ··· | ··· |
| 20.0 | 293.2 | 20.2 | ··· | ··· | 83.2[b] | 0.925 |
| 20.6* | 293.8 | ··· | 6.5[a] | 0.147 | ··· | ··· |
| 21.8* | 295.0 | ··· | ··· | ··· | 81.3[b] | 0.915 |
| 22.4* | 295.6 | ··· | 2.7[a] | 0.064 | ··· | ··· |
| 22.5* | 295.7 | ··· | 19.5[b] | 0.375 | ··· | ··· |
| 26.2* | 299.4 | ··· | ··· | ··· | 72.3[b] | 0.866 |
| 26.5* | 299.7 | ··· | 27.8[b] | 0.489 | ··· | ··· |
| 28.2* | 301.4 | ··· | ··· | ··· | 63.5[b] | 0.812 |
| 29.0* | 302.2 | ··· | 43.2[b] | 0.654 | ··· | ··· |
| 29.1* | 302.3 | ··· | ··· | ··· | 54.8[b] | 0.751 |

*Data extracted from the published graphs by the compilers.
[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium occurs at 292.0 K.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The solubility measurements were made with the equipment and in the manner described in Hoerr *et al.*[1] and Ralston *et al.*[2]

**Source and Purity of Materials:**
(1) Source not specified; purity not specified.
(2) Source not specified; commercial product; purified by vacuum distillation in a Stedman packed column; freezing point = 23.95 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. **9**, 102 (1944).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**
A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

**Variables:**
$T$/K = 287–300

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Mutual solubility of nitroethane (1) and 1-dodecanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 14.0 | 287.2 | ··· | ··· | 92.0 | 0.966 |
| 16.0 | 289.2 | ··· | ··· | 90.0 | 0.957 |
| 20.0 | 293.2 | 23.0 | 0.426 | 84.0 | 0.929 |
| 24.0 | 297.2 | 30.0 | 0.516 | 75.0 | 0.882 |
| 26.5 | 299.7 | 55.0 | 0.752 | 55.0 | 0.752 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The observations were made after vigorously shaking glass stoppered graduated tubes of about 15 mL capacity immersed in water baths in large Dewar flasks. The water was agitated with a rapid stream of air bubbles. The temperature was adjusted by adding small amounts of cooler or warmer water occasionally as required.

**Source and Purity of Materials:**
(1) Eastman Kodak Co.; distilled with 30 cm column with reflux; boiling point = 114 °C–115 °C; $n$(20 °C,D) = 1.3920, $\rho$(20 °C) = 1046.9 g·L$^{-1}$.
(2) Source not specified; purified by crystallization; melting point = 22.7 °C; $n$(24 °C,D) = 1.4410, $\rho$(24 °C) = 832.0 g·L$^{-1}$.

**Estimated Error:**
Not specified.

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**
E. F. Zhuravlev and L. F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10–7 (1968).

**Variables:**
$T$/K = 294–302

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Mutual solubility of nitroethane (1) and 1-dodecanol (2)

| | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 21.2 | 294.4 | 24.6 | 0.448 | ··· | ··· |
| 23.0 | 296.2 | ··· | ··· | 79.1 | 0.904 |
| 23.8 | 297.0 | 27.6 | 0.486 | ··· | ··· |
| 26.4 | 299.6 | 32.8 | 0.548 | ··· | ··· |
| 26.5 | 299.7 | ··· | ··· | 70.7 | 0.857 |
| 27.8 | 301.0 | 40.5 | 0.628 | ··· | ··· |
| 28.1 | 301.3 | ··· | ··· | 59.6 | 0.786 |
| 28.4 | 301.6 | 49.4 | 0.708 | ··· | ··· |
| 28.4 | 301.6 | 52.5 | 0.733 | 52.5 | 0.733 (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method (Alekseev[1]) was used.
No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; dried and distilled.
(2) Source not specified; purity not specified; dried and distilled.

**Estimated Error:**
Not specified.

**References:**
[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

## 3.31. Tridecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Tridecanoic acid; $C_{13}H_{26}O_2$; [638-53-9]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273–313

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Solubility of tridecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 1.4 | 1.4 | 0.005 |
| 10.0 | 283.2 | 2.1 | 2.1 | 0.007 |
| 20.0 | 293.2 | 4.5 | 4.3 | 0.016 |
| 30.0 | 303.2 | 17.3 | 14.8 | 0.057 |
| 40.0 | 313.2 | 9000 | 98.9 | 0.969 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used.
No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=41.76 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.32. Tetradecanenitrile

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Tetradecanenitrile; $C_{14}H_{27}N$; [629-63-0]

**Original Measurements:**
C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68–80 (1944).

**Variables:**
$T$/K=233–288

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The solubilities of tetradecanenitrile (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of tetradecanenitrile (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −40.0 | 233.2 | 1.0 | 1.0 | 0.004 |
| −26.7* | 246.5 | ··· | 1.8 | 0.006 |
| −20.0 | 253.2 | 3.1 | 3.0 | 0.011 |
| −15.9* | 257.3 | ··· | 4.5 | 0.017 |
| −7.7* | 265.5 | ··· | 10.0 | 0.038 |
| −4.4* | 268.8 | ··· | 14.1 | 0.056 |
| 0.0 | 273.2 | 32.7 | 24.6 | 0.105 |
| 0.2* | 273.4 | ··· | 25.5 | 0.109 |
| 4.7* | 277.9 | ··· | 44.0 | 0.220 |
| 10.0 | 283.2 | 207 | 67.4 | 0.426 |
| 15.1* | 288.3 | ··· | 87.5 | 0.715 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron-constantan thermocouple. As the nitrile crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing the tetradecanoic acid over aluminum oxide in the presence of ammonia at 673 °C; dried and purified by vacuum distillation in a Stedman packed column; freezing point=19.25 °C.

**Estimated Error:**
Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

## 3.33. Tetradecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Tetradecanoic acid; $C_{14}H_{28}O_2$; [544-63-8]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K=273–323

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility of tetradecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 0.3 | 0.3 | 0.001 |
| 10.0 | 283.2 | 0.5 | 0.5 | 0.002 |
| 20.0 | 293.2 | 1.2 | 1.2 | 0.003 |
| 30.0 | 303.2 | 3.3 | 3.2 | 0.011 |
| 40.0 | 313.2 | 10.7 | 9.7 | 0.034 |
| 50.0 | 323.2 | 1180 | 92.2 | 0.795 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Raltson;[2] freezing point=54.15 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.34. Tetradecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Tetradecanamide; $C_{14}H_{29}NO$; [638-58-4]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–373

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of tetradecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of tetradecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.3 | 0.3 | 0.001 |
| 30.0 | 303.2 | 0.5 | 0.5 | 0.002 |
| 34.5* | 307.7 | ··· | 0.7 | 0.002 |
| 50.0 | 323.2 | 2.0 | 2.0 | 0.007 |
| 51.8* | 325.0 | ··· | 2.1 | 0.007 |
| 70.0 | 343.2 | 7.5 | 7.0 | 0.024 |
| 75.5* | 348.7 | ··· | 11.4 | 0.041 |
| 83.5* | 356.7 | ··· | 30.0 | 0.124 |
| 88.0* | 361.2 | ··· | 48.8 | 0.239 |
| 90.0 | 363.2 | 142 | 58.7 | 0.319 |
| 93.2* | 366.4 | ··· | 73.6 | 0.479 |
| 98.2* | 371.4 | ··· | 89.7 | 0.742 |
| 100.0 | 373.2 | 1500 | 93.8 | 0.832 |

*The compilers extracted these data from the published graphs.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the tetradecanoic acid at 190–210 °C for 10–14 h; purified by recrystallization; freezing point = 105.1 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.35 1-Tetradecanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Tetradecanol; $C_{14}H_{30}O$; [112-72-1]

**Original Measurements:**
C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267–80 (1944).

**Variables:**
$T$/K = 283–309

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of nitroethane (1) and 1-tetradecanol (2) in mass percent including the region of immiscible solution over the temperature range were presented in graphical form and in a table.

Mutual solubility of nitroethane (1) and 1-tetradecanol (2)

| | | | Alcohol-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_1$ | $x_1$ (compilers) | $100\ w_1$ | $x_1$ (compilers) |
| 10.0 | 283.2 | 0.1 | ··· | ··· | 99.9[a] | 0.9996 |
| 19.2* | 292.4 | ··· | ··· | ··· | 98.3[a] | 0.994 |
| 20.0 | 293.2 | 1.9 | ··· | ··· | 98.1[a] | 0.993 |
| 26.1* | 299.3 | ··· | ··· | ··· | 94.2[a] | 0.979 |
| 29.0* | 302.2 | ··· | ··· | ··· | 89.0[a] | 0.958 |
| 30.0 | 303.2 | 14.5 | ··· | ··· | 87.3[a] | 0.951 |
| 31.6* | 304.8 | ··· | ··· | ··· | 80.4[a] | 0.921 |
| 32.6* | 305.8 | ··· | 20.3[a] | 0.421 | ··· | ··· |
| 32.7* | 305.9 | ··· | ··· | ··· | 71.6[b] | 0.878 |
| 33.3* | 306.5 | ··· | 30.7[b] | 0.558 | ··· | ··· |
| 33.7* | 307.0 | ··· | ··· | ··· | 67.2[b] | 0.854 |
| 33.7* | 307.0 | ··· | 12.3[a] | 0.286 | ··· | ··· |
| 34.6* | 307.8 | ··· | 41.6[b] | 0.670 | ··· | ··· |
| 34.9* | 308.1 | ··· | ··· | ··· | 54.8[b] | 0.776 |
| 35.7* | 308.9 | ··· | 5.2[a] | 0.135 | ··· | ··· |

*The compilers extracted these data from the published graphs.
[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium occurs at 295.4 K.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The solubility measurements were made with the equipment and in the manner described in Hoerr *et al.*[1] and Ralston *et al.*[2]

**Source and Purity of Materials:**
(1) Source not specified; purity not specified.
(2) Prepared by catalytic hydrogenation of methyl myristate; purified by vacuum distillation; freezing point = 38.26 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. **9**, 102 (1944).

## 3.36. Pentadecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Pentadecanoic acid; $C_{15}H_{30}O_2$; [1002-84-2]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K = 273–323

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Solubility of pentadecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 0.0 | 273.2 | 0.1 | 0.1 | 0.0003 |
| 10.0 | 283.2 | 0.2 | 0.2 | 0.0006 |
| 20.0 | 293.2 | 0.7 | 0.7 | 0.0022 |
| 30.0 | 303.2 | 2.4 | 2.3 | 0.0074 |
| 40.0 | 313.2 | 10.2 | 9.3 | 0.0308 |
| 50.0 | 323.2 | 2460 | 96.1 | 0.8843 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=52.54 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.37. N-Phenyldecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) N-Phenyldecanamide; $C_{16}H_{25}NO$; [15473-32-2]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–336

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**
The solubilities of *N*-phenyldecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of *N*-phenyldecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 14.0 | 12.3 | 0.041 |
| 16.7* | 289.9 | ··· | 13.7 | 0.046 |
| 30.0 | 303.2 | 21.8 | 17.9 | 0.062 |
| 33.8* | 307.0 | ··· | 20.0 | 0.071 |
| 41.3* | 314.5 | ··· | 27.5 | 0.103 |
| 43.8* | 317.0 | ··· | 35.3 | 0.142 |
| 50.0 | 323.2 | 133 | 57.1 | 0.288 |
| 50.4* | 323.6 | ··· | 57.6 | 0.292 |
| 59.3* | 332.5 | ··· | 82.5 | 0.589 |
| 62.7* | 335.9 | ··· | 88.7 | 0.704 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained by heating of decanoic acid with redistilled aniline at 150 °C–170 °C for 2–3 h; purified by recrystallization; freezing point=69.5 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.38. Hexadecanenitrile

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexadecanenitrile; $C_{16}H_{31}N$; [629-79-8]

**Original Measurements:**
C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68–80 (1944).

**Variables:**
$T$/K=233–303

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

The solubilities of hexadecanenitrile (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of hexadecanenitrile (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −40.0 | 233.2 | 0.1 | 0.1 | 0.0003 |
| −20.0 | 253.2 | 1.0 | 1.0 | 0.0032 |
| −18.4* | 254.8 | ··· | 1.1 | 0.0035 |
| −7.1* | 266.1 | ··· | 3.5 | 0.011 |
| 0.0 | 273.2 | 6.6 | 6.2 | 0.021 |
| 1.0* | 274.2 | ··· | 6.8 | 0.023 |
| 7.3* | 280.5 | ··· | 12.1 | 0.042 |
| 10.0 | 283.2 | 20.2 | 16.8 | 0.060 |
| 12.6* | 285.8 | ··· | 24.7 | 0.094 |
| 16.4* | 289.6 | ··· | 40.0 | 0.174 |
| 20.0 | 293.2 | 127 | 55.9 | 0.286 |
| 21.8* | 295.0 | ··· | 63.6 | 0.356 |
| 24.8* | 298.0 | ··· | 77.5 | 0.521 |
| 26.4* | 299.6 | ··· | 84.1 | 0.626 |
| 30.0 | 303.2 | 2850 | 96.6 | 0.900 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron-constantan thermocouple. As the nitrile crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing the hexadecanoic acid over aluminum oxide in the presence of ammonia at 400 °C; dried and purified by vacuum distillation in a Stedman packed column; freezing point=31.40 °C.

**Estimated Error:**
Temperature: ±0.4 K (below 248 K), ±0.2 K (above 248 K).

## 3.39. Hexadecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Hexadecanoic acid; $C_{16}H_{32}O_2$; [57-10-3]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K=293–333

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility of hexadecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 20.0 | 293.2 | 0.1 | 0.1 | 0.0003 |
| 30.0 | 303.2 | 0.7 | 0.7 | 0.0021 |
| 40.0 | 313.2 | 2.6 | 2.5 | 0.0075 |
| 50.0 | 323.2 | 10.0 | 9.1 | 0.0284 |
| 60.0 | 333.2 | 1650 | 94.3 | 0.8286 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=62.82 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.40. Hexadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Hexadecanamide; $C_{16}H_{33}NO$; [629-54-9]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1953).

**Variables:**
$T$/K = 283–373

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of hexadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of hexadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.2 | 0.2 | 0.0006 |
| 30.0 | 303.2 | 0.3 | 0.3 | 0.001 |
| 45.5* | 318.7 | ··· | 0.8 | 0.002 |
| 50.0 | 323.2 | 0.9 | 0.9 | 0.003 |
| 52.8* | 326.0 | ··· | 1.6 | 0.005 |
| 70.0 | 343.2 | 7.5 | 7.0 | 0.022 |
| 70.5* | 343.7 | ··· | 7.3 | 0.023 |
| 80.5* | 353.7 | ··· | 24.1 | 0.085 |
| 88.4* | 361.6 | ··· | 60.0 | 0.306 |
| 90.0 | 363.2 | 208 | 67.5 | 0.379 |
| 92.5* | 365.7 | ··· | 76.6 | 0.490 |
| 96.4* | 369.6 | ··· | 85.0 | 0.625 |
| 99.6* | 372.8 | ··· | 90.8 | 0.744 |
| 100.0 | 373.2 | 1075 | 91.5 | 0.760 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the hexadecanoic acid at 190 °C–210 °C for 10–14 h; purified by recrystallization; freezing point = 107.0 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.41. 1-Hexadecanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Hexadecanol; $C_{16}H_{34}O$; [36653-82-4]

**Original Measurements:**
C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267–80 (1944).

**Variables:**
$T$/K = 293–319

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 1-hexadecanol (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 1-hexadecanol (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 20.0 | 293.2 | 0.1 | 0.1 | 0.0003 |
| 28.8* | 302.0 | ··· | 1.2 | 0.004 |
| 30.0 | 303.2 | 1.6 | 1.4 | 0.005 |
| 38.4* | 311.6 | ··· | 9.1 | 0.030 |
| 40.0 | 313.2 | 13.4 | 11.8 | 0.040 |
| 40.5* | 313.7 | ··· | 13.0 | 0.044 |
| 43.5* | 316.7 | ··· | 25.9 | 0.098 |
| 44.3* | 317.5 | ··· | 38.2 | 0.161 |
| 44.8* | 318.0 | ··· | 63.9 | 0.354 |
| 45.0* | 318.2 | ··· | 77.0 | 0.509 |
| 45.7* | 318.9 | ··· | 85.7 | 0.650 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubility measurements were made with the equipment and in the manner described in Hoerr *et al.*[1] and Ralston *et al.*[2]

**Source and Purity of Materials:**
(1) Source not specified; purity not specified.
(2) Source not specified; commerical product; purified by recrystallization; freezing point = 49.62 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. **9**, 102 (1944).

## 3.42. Heptadecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Heptadecanoic acid; $C_{17}H_{34}O_2$ ; [506-12-7]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K=303–333

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**
Solubility of heptadecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 30.0 | 303.2 | 0.2 | 0.2 | 0.001 |
| 40.0 | 313.2 | 1.9 | 1.8 | 0.005 |
| 50.0 | 323.2 | 9.6 | 8.8 | 0.026 |
| 60.0 | 333.2 | 4250 | 97.7 | 0.922 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*;[1] dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=60.94 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.43. N-Phenyldodecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) N-Phenyldodecanamide; $C_{18}H_{29}NO$; [3430-95-3]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K=283–344

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**
The solubilities of N-phenyldodecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N-phenyldodecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 6.0 | 5.7 | 0.016 |
| 13.8* | 287.0 | ··· | 5.9 | 0.017 |
| 30.0 | 303.2 | 8.5 | 7.8 | 0.023 |
| 31.0* | 304.2 | ··· | 8.2 | 0.024 |
| 45.9* | 319.1 | ··· | 14.0 | 0.042 |
| 50.0 | 323.2 | 22.3 | 18.2 | 0.057 |
| 53.6* | 326.8 | ··· | 26.6 | 0.090 |
| 58.4* | 331.6 | ··· | 50.0 | 0.214 |
| 64.5* | 337.7 | ··· | 74.1 | 0.438 |
| 70.0 | 343.2 | 720 | 87.8 | 0.662 |
| 70.3* | 343.5 | ··· | 88.2 | 0.671 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Raltston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained by heating of dodecanoic acid with redistilled aniline at 150 °C–170 °C for 2–3 h; purified by recrystallization; freezing point=77.2 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.44. 9,12-Octadecadienoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 9,12-Octadecadienoic acid; $C_{18}H_{32}O_2$; [60-33-3]

**Original Measurements:**
C. W. Hoerr and H. J. Harwood, J. Phys. Chem. **56**, 1068–73 (1952).

**Variables:**
$T$/K = 243–275

**Prepared By:**
V. P. Sazonov and N. I. Lisov

### Experimental Data

The solubilities of 9,12-octadecadienoic acid (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 9,12-octadecadienoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −30.0 | 243.2 | 0.4[a] | 0.4 | 0.001 |
| −20.0 | 253.2 | 2.1[a] | 2.1 | 0.006 |
| −10.0 | 263.2 | 8.3[b] | 7.7 | 0.022 |
| 0.0 | 273.2 | 34.2[b] | 25.5 | 0.084 |
| 1.5 | 274.7 | ··· | ··· | ··· (UCST) |

[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of acid were determined by weighing 2–5 g portions of the acid into 2 cm×15 cm Pyrex test tubes which were fitted with a Nichrome stirrer and a thermocouple well, the test tube being inserted into a larger tube which served as an air bath. Upon successive additions of weighed amounts of solvent, the solubilities were determined by measuring the temperatures at which crystals precipitated and dissolved upon alternately cooling and heating the systems in an acetone-dry ice bath or water bath as required.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; distilled.
(2) Chemical Division, Armour and Co.; purified by stepwise fractional crystallization and vacuum distilled a short Vigreux column; melting point = −5.2 °C, $n$(20 °C,D) = 1.4703.

**Estimated Error:**
Temperature: ±0.1 K.

## 3.45. cis-9-Octadecenoic acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) cis-9-Octadecenoic acid; $C_{18}H_{34}O_2$; [112-80-1]

**Original Measurements:**
C. W. Hoerr and H. J. Harwood, J. Phys. Chem. **56**, 1068–73 (1952).

**Variables:**
$T$/K = 233–305

**Prepared By:**
V. P. Sazonov and N. I. Lisov

### Experimental Data

The solubilities of cis-9-octadecenoic acid (2) in nitroethane (1) in mole fraction including the region of immiscible solutions over the temperature range were presented in graphical form and in a table.

Solubility of cis-9-octadecenoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −40.0 | 233.2 | 0.2[a] | 0.2 | 0.001 |
| −30.0 | 243.2 | 0.8[a] | 0.8 | 0.002 |
| −20.0 | 253.2 | 1.3[a] | 1.3 | 0.003 |
| −10.0 | 263.2 | 2.2[a] | 2.1 | 0.006 |
| 0.0 | 273.2 | 3.4[a] | 3.3 | 0.009 |
| 10.0 | 283.2 | 8.7[b] | 8.0 | 0.023 |
| 20.0 | 293.2 | 14.3[b] | 12.5 | 0.037 |
| 31.7 | 304.9 | ··· | ··· | ··· (UCST) |

[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of acid were determined by weighing 2–5 g portions of the acid into 2 cm×15 cm Pyrex test tubes which were fitted with a Nichrome stirrer and a thermocouple well, the test tube being inserted into a larger tube which served as an air bath. Upon successive additions of weighed amounts of solvent, the solubilities were determined by measuring the temperatures at which crystals precipitated and dissolved upon alternately cooling and heating the systems in an acetone-dry ice bath or water bath as required.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and distilled.
(2) Prepared from high quality oil by saponification; purified by recrystallization and by vacuum distillation in packed column; melting point = 16.30 °C, $n$(20 °C,D) = 1.4599.

**Estimated Error:**
Temperature: ±0.1 K.

## 3.46. Octadecanenitrile

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Octadecanenitrile; $C_{18}H_{35}N$; [638-65-3]

**Original Measurements:**
C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68–80 (1944).

**Variables:**
$T$/K=253–310

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of octadecanenitrile (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of octadecanenitrile (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| −20.0 | 253.2 | 0.1 | 0.1 | 0.0003 |
| −4.9* | 268.3 | ··· | 0.3 | 0.0009 |
| 0.0 | 273.2 | 0.8 | 0.8 | 0.0023 |
| 4.3* | 277.5 | ··· | 1.8 | 0.0052 |
| 10.0 | 283.2 | 3.9 | 3.8 | 0.011 |
| 12.5* | 285.7 | ··· | 5.3 | 0.016 |
| 17.5* | 290.7 | ··· | 10.0 | 0.031 |
| 20.0 | 293.2 | 17.8 | 15.9 | 0.048 |
| 20.7* | 293.9 | ··· | 17.5 | 0.057 |
| 24.5* | 297.7 | ··· | 33.2 | 0.123 |
| 29.9* | 303.1 | ··· | 57.3 | 0.275 |
| 30.0 | 303.2 | 137 | 57.8 | 0.279 |
| 32.5* | 305.7 | ··· | 69.5 | 0.392 |
| 36.4* | 309.6 | ··· | 85.9 | 0.633 |

*These data were extracted by the compilers from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Solution temperatures were determined by cooling 3–5 g portions of solution in 1 cm×15 cm test tubes, which were placed in an air bath. The latter was immersed in an acetone bath, which was cooled with solid carbon dioxide. Temperature within the samples was measured by means of a potentiometer with an iron-constantan thermocouple. As the nitrile crystallized from solution upon cooling, the temperature of the air bath was raised gradually until the mixtures redissolved.

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing the octadecanoic acid over aluminum oxide in the presence of ammonia at 673 K; purified by several crystallization; freezing point=40.88 °C.

**Estimated Error:**
Temperature: ±0.2 K and ±0.4 K (below 248 K).

## 3.47. Octadecanoic Acid

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Octadecanoic acid; $C_{18}H_{36}O_2$ ; [57-11-4]

**Original Measurements:**
C. W. Hoerr and A. W. Ralston, J. Org. Chem. **9**, 329–37 (1944).

**Variables:**
$T$/K=313–333

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility of octadecanoic acid (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\ g_1$ | $100\ w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 40.0 | 313.2 | 0.3 | 0.3 | 0.001 |
| 50.0 | 323.2 | 2.7 | 2.6 | 0.007 |
| 60.0 | 333.2 | 14.0 | 12.3 | 0.036 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method, as described in Hoerr *et al.*[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purified according to Hoerr *et al.*;[1] dried and twice distilled.
(2) Source not specified; purified according to Pool and Ralston;[2] freezing point=69.32 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]W. O. Pool and A. W. Ralston, Ind. Eng. Chem. **34**, 1104 (1942).

## 3.48. Octadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Octadecanamide; $C_{18}H_{37}NO$; [124-26-5]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–376

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of octadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of octadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.1 | 0.1 | 0.0003 |
| 30.0 | 303.2 | 0.2 | 0.2 | 0.0005 |
| 46.2* | 319.4 | ··· | 0.4 | 0.001 |
| 50.0 | 323.2 | 0.5 | 0.5 | 0.001 |
| 55.1* | 328.3 | ··· | 1.1 | 0.003 |
| 70.0 | 343.2 | 5.2 | 4.9 | 0.014 |
| 70.3* | 343.5 | ··· | 5.0 | 0.014 |
| 80.8* | 354.0 | ··· | 15.4 | 0.046 |
| 85.9* | 359.1 | ··· | 29.1 | 0.098 |
| 90.0 | 363.2 | 93.0 | 48.2 | 0.198 |
| 91.2* | 364.4 | ··· | 55.0 | 0.245 |
| 96.7* | 369.9 | ··· | 76.5 | 0.463 |
| 100.0 | 373.2 | 610[a] | 85.9 | 0.617 |
| 102.5* | 375.7 | ··· | 91.1 | 0.731 |

*These data were extracted by the compilers from the published graphs.
[a]Recorded as 61.0 in original. Value corrected by compilers based on graphical data.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by passing of ammonia through the octadecanoic acid at 190 °C–210 °C for 10 to 14 h; purified by recrystallization; freezing point = 109.7 °C.

**Estimated Error:**
Temperature: control ± 0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.49. 1-Octadecanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Octadecanol; $C_{18}H_{38}O$; [112-92-5]

**Original Measurements:**
C. W. Hoerr, H. J. Harwood, and A. W. Ralston, J. Org. Chem. **9**, 267–80 (1944).

**Variables:**
$T$/K = 303–327

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of 1-octadecanol (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 1-octadecanol (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 30.0 | 303.2 | 0.1 | 0.1 | 0.0003 |
| 36.1* | 309.3 | ··· | 1.0 | 0.003 |
| 40.0 | 313.2 | 2.7 | 2.6 | 0.007 |
| 40.7* | 313.9 | ··· | 3.3 | 0.009 |
| 43.9* | 317.1 | ··· | 6.7 | 0.020 |
| 48.5* | 321.7 | ··· | 15.5 | 0.048 |
| 50.0 | 323.2 | 25.4 | 20.3 | 0.066 |
| 50.9* | 324.1 | ··· | 26.6 | 0.091 |
| 51.5* | 324.7 | ··· | 32.6 | 0.118 |
| 52.2* | 325.4 | ··· | 47.0 | 0.198 |
| 52.5* | 325.7 | ··· | 67.7 | 0.368 |
| 53.8* | 327.0 | ··· | 85.7 | 0.625 |

*The compilers extracted these data from the published graphs.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubility measurements were made with the equipment and in the manner described in Hoerr *et al.*[1] and Ralston *et al.*[2]

**Source and Purity of Materials:**
(1) Source not specified; purity not specified.
(2) Prepared by catalytic hydrogenation of ethyl stearate; purified by vacuum distillation; freezing point = 57.98 °C.

**Estimated Error:**
Not specified.

**References:**
[1]C. W. Hoerr, E. F. Binkerd, W. O. Pool, and A. W. Ralston, J. Org. Chem. **9**, 68 (1944).
[2]A. W. Ralston, C. W. Hoerr, W. O. Pool, and H. J. Harwood, J. Org. Chem. **9**, 102 (1944).

## 3.50. 10-Nonadecanone

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 10-Nonadecanone; $C_{19}H_{38}O$; [504-57-4]

**Original Measurements:**
F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. **8**, 344–57 (1943).

**Variables:**
$T$/K = 293–327

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 10-nonadecanone (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 10-nonadecanone (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 20.0 | 293.2 | 1.6 | 1.6 | 0.004 |
| 23.3* | 296.5 | ··· | 1.9 | 0.005 |
| 26.9* | 300.1 | ··· | 2.7 | 0.007 |
| 36.7* | 310.0 | ··· | 9.3 | 0.027 |
| 38.9* | 312.1 | ··· | 13.6 | 0.040 |
| 40.0 | 313.2 | 19.8 | 16.5 | 0.050 |
| 42.6* | 315.8 | ··· | 28.6 | 0.096 |
| 45.6* | 318.8 | ··· | 52.4 | 0.226 |
| 48.9* | 322.1 | ··· | 72.5 | 0.412 |
| 50.0 | 323.2 | 350 | 77.8 | 0.482 |
| 52.6* | 325.8 | ··· | 87.3 | 0.646 |
| 53.5* | 326.7 | ··· | 90.4 | 0.715 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Harwood *et al.*[1] and Raltston *et al.*[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketoester by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several recrystallization from ethanol; freezing point = 57.8 °C.

**Estimated Error:**
Temperature: ±0.2 K.

**References:**
[1]H. J. Harwood, A. W. Ralston, and W. M. Selby, J. Am. Chem. Soc. **63**, 1916 (1941).
[2]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).

## 3.51. N,N-Diphenyldecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) N,N-Diphenyldecanamide; $C_{22}H_{29}NO$; [153736-38-0]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–314

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of N,N-diphenyldecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N,N-diphenyldecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 57.0 | 36.3 | 0.117 |
| 14.2* | 287.4 | ··· | 40.9 | 0.138 |
| 22.9* | 296.1 | ··· | 59.5 | 0.254 |
| 30.0 | 303.2 | 310 | 75.6 | 0.420 |
| 31.6* | 304.8 | ··· | 78.0 | 0.451 |
| 40.6* | 313.8 | ··· | 92.1 | 0.730 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the decanoyl chloride with diphenylamine for 2–4 h at 135 °C–145 °C; purified by recrystallization; freezing point = 47.5 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.52. N-Phenylhexadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) N-Phenylhexadecanamide; $C_{22}H_{37}NO$; [6832-98-0]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–356

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of N-phenylhexadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N-phenylhexadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.5 | 0.5 | 0.001 |
| 30.0 | 303.2 | 0.8 | 0.8 | 0.002 |
| 49.5* | 322.7 | ··· | 3.2 | 0.007 |
| 50.0 | 323.2 | 3.4 | 3.3 | 0.008 |
| 64.4* | 337.6 | ··· | 10.9 | 0.027 |
| 68.8* | 342.0 | ··· | 21.5 | 0.058 |
| 70.0 | 343.2 | 41.8 | 29.5 | 0.087 |
| 72.0* | 345.2 | ··· | 40.4 | 0.133 |
| 74.8* | 348.0 | ··· | 57.3 | 0.233 |
| 79.1* | 352.3 | ··· | 70.0 | 0.346 |
| 82.3* | 355.5 | ··· | 84.3 | 0.549 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained by heating of hexadecanoic acid with redistilled aniline at 150 °C–170 °C for 2–3 h; purified by recrystallization; freezing point = 90.2 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.53. 12-Tricosanone

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 12-Tricosanone; $C_{23}H_{46}O$; [540-09-0]

**Original Measurements:**
F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. **8**, 344–57 (1943).

**Variables:**
$T$/K = 293–339

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 12-tricosanone (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 12-tricosanone (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 20.0 | 293.2 | 0.5 | 0.5 | 0.001 |
| 25.7* | 298.9 | ··· | 0.9 | 0.002 |
| 40.0 | 313.2 | 1.5 | 1.5 | 0.003 |
| 40.7* | 313.9 | ··· | 1.8 | 0.004 |
| 48.0* | 321.2 | ··· | 4.8 | 0.011 |
| 50.0 | 323.2 | 7.5 | 7.0 | 0.016 |
| 53.6* | 326.8 | ··· | 13.8 | 0.034 |
| 55.6* | 328.8 | ··· | 25.9 | 0.072 |
| 58.6* | 331.8 | ··· | 59.0 | 0.242 |
| 60.0 | 333.2 | 230 | 69.7 | 0.338 |
| 62.2* | 335.4 | ··· | 80.0 | 0.470 |
| 66.2* | 339.4 | ··· | 92.3 | 0.727 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketoesters by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several recrystallization from ethanol; freezing point = 69.3 °C.

**Estimated Error:**
Temperature: ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.54. Tricosane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Tricosane; $C_{23}H_{48}$; [638-67-5]

**Original Measurements:**
V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel **8**, 9–13 (1970).

**Variables:**
$T$/K = 303–356

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual solubility of nitroethane (1) and tricosane (2) in mass percent including the region of immiscible solutions over the temperature range were presented in a graphical form. The data in this table were sent to compilers by the authors upon his request.

Mutual solubility of nitroethane (1) and tricosane (2)

| | | Hydrocarbon-rich phase | | Nitroethane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 30.0[a] | 303.2 | ··· | ··· | 99.3 | 0.998 |
| 40.0[a] | 313.2 | ··· | ··· | 98.5 | 0.997 |
| 44.2[a] | 317.5 | ··· | ··· | 98.1 | 0.996 |
| 47.7[a] | 320.9 | 18.0 | 0.487 | ··· | ··· |
| 52.5[b] | 325.7 | ··· | ··· | 97.2 | 0.993 |
| 53.0[b] | 326.2 | 20.0 | 0.520 | ··· | ··· |
| 62.2[b] | 335.4 | 22.8 | 0.561 | ··· | ··· |
| 62.4[b] | 335.6 | ··· | ··· | 95.8 | 0.990 |
| 72.2[b] | 345.4 | 25.3 | 0.594 | 94.3 | 0.986 |
| 81.3[b] | 354.5 | 27.0 | 0.615 | ··· | ··· |
| 82.3[b] | 355.5 | ··· | ··· | 92.2 | 0.981 |

[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium is realized at 320.7 K. The upper critical solution temperature was reported to be above 90 °C.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; boiling point = 383.8 °C, melting point = 47.7 °C.

**Estimated Error:**
Not reported.

## 3.55. N,N-Diphenyldodecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) N,N-Diphenyldodecanamide; $C_{24}H_{33}NO$; [153736-39-1]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–323

**Prepared By:**
N. I. Lisov; V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of N,N-diphenyldodecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N,N-diphenyldodecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 29.0 | 22.5 | 0.059 |
| 15.0* | 288.2 | ··· | 27.2 | 0.074 |
| 25.8* | 299.0 | ··· | 44.6 | 0.147 |
| 30.0 | 303.2 | 118 | 54.1 | 0.202 |
| 35.9* | 309.1 | ··· | 66.4 | 0.297 |
| 45.5* | 318.7 | ··· | 84.1 | 0.530 |
| 50.0 | 323.2 | 1100 | 91.7 | 0.702 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the dodecanoyl chloride with diphenylamine for 2–4 h at 135 °C–145 °C; purified by recrystallization; freezing point = 57 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.56. N-Phenyloctadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) N-Phenyloctadecanamide; $C_{24}H_{41}NO$; [637-54-7]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–363

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of N-phenyloctadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N-phenyloctadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 0.4 | 0.4 | 0.0008 |
| 30.0 | 303.2 | 0.6 | 0.6 | 0.0013 |
| 44.7* | 317.9 | ··· | 1.4 | 0.003 |
| 50.0 | 323.2 | 2.0 | 2.0 | 0.004 |
| 64.6* | 337.8 | ··· | 6.9 | 0.015 |
| 70.0 | 343.2 | 14.7 | 12.8 | 0.030 |
| 70.5* | 343.7 | ··· | 13.1 | 0.031 |
| 74.5* | 347.7 | ··· | 28.0 | 0.075 |
| 78.9* | 352.1 | ··· | 54.8 | 0.202 |
| 86.1* | 359.3 | ··· | 82.0 | 0.488 |
| 87.7* | 360.9 | ··· | 87.1 | 0.585 |
| 90.0 | 363.2 | 1060 | 91.4 | 0.689 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by addition of aniline to stearoyl chloride at 50 °C; purified by recrystallization; freezing point=94.9 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.57. 14-Heptacosanone

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 14-Heptacosanone; $C_{27}H_{54}O$; [542-50-7]

**Original Measurements:**
F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. **8**, 344–57 (1943).

**Variables:**
$T$/K = 293–346

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 14-heptacosanone (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 14-heptacosanone (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 20.0 | 293.2 | 0.1 | 0.1 | 0.0002 |
| 40.0 | 313.2 | 0.2 | 0.2 | 0.0004 |
| 42.3* | 315.5 | ··· | 0.3 | 0.0005 |
| 50.0 | 323.2 | 0.9 | 0.9 | 0.0017 |
| 51.4* | 324.6 | ··· | 1.2 | 0.002 |
| 60.0 | 333.2 | 5.6 | 5.3 | 0.011 |
| 61.8* | 335.0 | ··· | 7.6 | 0.015 |
| 65.5* | 338.7 | ··· | 20.7 | 0.047 |
| 66.6* | 339.8 | ··· | 49.5 | 0.157 |
| 68.5* | 341.7 | ··· | 70.1 | 0.308 |
| 72.9* | 346.1 | ··· | 88.8 | 0.601 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketoesters by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point=77.2 °C.

**Estimated Error:**
Temperature: ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.58. N,N-Diphenylhexadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) N,N-Diphenylhexadecanamide; $C_{28}H_{41}NO$; [141650-17-1]

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–334

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of N,N-diphenylhexadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N,N-diphenylhexadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 16.1 | 13.9 | 0.029 |
| 13.2* | 286.4 | ··· | 15.0 | 0.032 |
| 27.9* | 301.1 | ··· | 20.9 | 0.046 |
| 30.0 | 303.2 | 29.0 | 22.5 | 0.051 |
| 37.7* | 310.9 | ··· | 31.3 | 0.077 |
| 49.4* | 322.6 | ··· | 61.8 | 0.230 |
| 50.0 | 323.2 | 179 | 64.2 | 0.249 |
| 60.6* | 333.8 | ··· | 86.9 | 0.550 |

*The compilers extracted these data from the published graphs.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the hexadecanoyl chloride with diphenylamine for 2–4 h at 135 °C–145 °C; purified by recrystallization; freezing point = 69.5 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.59. N,N-Diphenyloctadecanamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) N,N-Diphenyloctadecanamide; $C_{30}H_{45}NO$

**Original Measurements:**
A. W. Ralston, C. W. Hoerr, and W. O. Pool, J. Org. Chem. **8**, 473–88 (1943).

**Variables:**
$T$/K = 283–343

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubilities of N,N-diphenyloctadecanamide (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of N,N-diphenyloctadecanamide (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 10.0 | 283.2 | 10.9 | 9.8 | 0.019 |
| 11.8* | 285.0 | ··· | 10.2 | 0.020 |
| 27.3* | 300.5 | ··· | 14.4 | 0.028 |
| 30.0 | 303.2 | 17.8 | 15.1 | 0.030 |
| 41.6* | 314.8 | ··· | 25.0 | 0.054 |
| 50.0 | 323.2 | 92.0 | 47.9 | 0.137 |
| 50.7* | 323.9 | ··· | 48.7 | 0.141 |
| 58.8* | 332.0 | ··· | 73.9 | 0.328 |
| 65.7* | 338.9 | ··· | 90.0 | 0.608 |
| 70.0 | 343.2 | 3100 | 96.9 | 0.843 |

*The compilers extracted these data from the published graphs.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Prepared by heating the octadecanoyl chloride with diphenylamine for 2–4 h at 135 °C–145 °C; purified by crystallization; freezing point = 72.3 °C.

**Estimated Error:**
Temperature: control ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.60. 16-Hentricontanone

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 16-Hentricontanone; $C_{31}H_{62}O$; [502-73-8]

**Original Measurements:**
F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. **8**, 344–57 (1943).

**Variables:**
$T$/K = 313–354

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 16-hentricontanone (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 16-hentricontanone (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 40.0 | 313.2 | <0.1 | <0.1 | <0.0002 |
| 50.0 | 323.2 | 0.2 | 0.2 | 0.0003 |
| 57.3* | 330.5 | ··· | 0.9 | 0.0015 |
| 60.0 | 333.2 | 1.0 | 1.0 | 0.0017 |
| 68.9* | 342.1 | ··· | 4.6 | 0.008 |
| 72.6* | 345.8 | ··· | 10.4 | 0.019 |
| 73.6* | 346.8 | ··· | 24.6 | 0.052 |
| 74.5* | 347.7 | ··· | 60.0 | 0.200 |
| 77.3* | 350.5 | ··· | 81.1 | 0.417 |
| 80.0 | 353.2 | 965 | 90.6 | 0.616 |
| 80.3* | 353.5 | ··· | 91.0 | 0.624 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketoesters by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point = 83.7 °C.

**Estimated Error:**
Temperature: ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.61. 18-Pentatriacontanone

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 18-Pentatriacontanone; $C_{35}H_{70}O$; [504-53-0]

**Original Measurements:**
F. M. Garland, C. W. Hoerr, W. O. Pool, and A. W. Ralston, J. Org. Chem. **8**, 344–57 (1943).

**Variables:**
$T$/K = 323–358

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubilities of 18-pentatriacontanone (2) in nitroethane (1) in mass percent over the temperature range were presented in graphical form and in a table.

Solubility of 18-pentatriacontanone (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2/100\,g_1$ | $100\,w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| 50.0 | 323.2 | <0.1 | <0.1 | <0.0001 |
| 60.0 | 333.2 | 0.2 | 0.2 | 0.0003 |
| 62.3* | 335.5 | ··· | 0.3 | 0.0004 |
| 70.0* | 343.2 | ··· | 1.3 | 0.002 |
| 76.2* | 349.4 | ··· | 5.7 | 0.009 |
| 79.1* | 352.3 | ··· | 15.6 | 0.027 |
| 79.5* | 352.7 | ··· | 37.1 | 0.080 |
| 79.9* | 353.1 | ··· | 58.7 | 0.174 |
| 80.0 | 353.2 | 150 | 60.0 | 0.182 |
| 80.9* | 354.1 | ··· | 72.1 | 0.277 |
| 84.4* | 357.6 | ··· | 89.1 | 0.548 |

*The compilers extracted these data from the published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubilities of (2) in (1) were determined in sealed tubes by the method and apparatus described in Ralston *et al.*[1] and Hoerr and Ralston.[2]

**Source and Purity of Materials:**
(1) Source not specified; best grade reagent; dried and twice distilled.
(2) Obtained from the ketoesters by hydrolyzing the latter with 5% alcoholic potassium hydroxide; purified by several crystallizations from ethanol; freezing point = 88.7 °C.

**Estimated Error:**
Temperature: ±0.2 K.

**References:**
[1]A. W. Ralston, C. W. Hoerr, and E. J. Hoffman, J. Am. Chem. Soc. **64**, 1516 (1942).
[2]C. W. Hoerr and A. W. Ralston, J. Am. Chem. Soc. **64**, 2824 (1942).

## 3.62. Oils

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Oils

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (4), 26–8 (1968).

**Variables:**
$T$/K = 326–389

**Prepared By:**
N. V. Sazonov

**Experimental Data**

Solubility temperatures of nitroethane (1) and oil (2) mixtures ratio 3:1

| Oil | Freezing point oil/°C | Kinematic viscosity oil/cS | $t$/°C | $T$/K (compiler) |
|---|---|---|---|---|
| Diesel fuel | −56 | 8.05 (20 °C) | 52.5 | 325.7 |
| Distillate oil | −45.5 | 7.84 (50 °C) | 75.5 | 348.7 |
| Distillate oil | −33 | 16.05 (50 °C) | 88.0 | 361.2 |
| Distillate oil | −27 | 6.28 (100 °C) | 97.0 | 370.2 |
| Residual oil | −18 | 20.55 (100 °C) | 115.5[a] | 388.7 |

[a]The data were determined by extrapolation of the oil solubility curve in a mixture of nitroethane and toluene.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Prepared from Tuimazin crude oil.

**Estimated Error:**
Not specified.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 3.63. Oil Fraction of Tuimazin Crude

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Oil fraction of Tuimazin crude

**Original Measurements:**
V. V. Polshinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9–13 (1970).

**Variables:**
$T$/K = 279–377

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Values of critical solution temperatures of nitroethane (1) and stocks of fractions of Tuimazin crude (2) are presented over the temperature range in graphical form.

Mean values of critical solution temperatures of nitroethane (1) and stocks of oil fraction of Tuimazin crude (2)

| Stock of oil fraction | $d$(20 °C,4 °C) | $n$(20 °C,D) | $t$/°C | $T$/K (compilers) |
|---|---|---|---|---|
| Heavily aromatics | 1.0232–1.0479 | 1.5787–1.5979 | 6 | 279 |
| Mean aromatics | 0.9706–0.9921 | 1.5430–1.5623 | 30 | 303 |
| Light aromatics | 0.9176 | 1.5090 | 64 | 337 |
| Paraffin–naphthenes | 0.8195–0.8667 | 1.4320*–1.4756 | 104 | 377 |

*$n$(70 °C,D)

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Bondarev and Kozlov[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified; $n$(20 °C,D) = 1.3919; $d$(20 °C,4 °C) = 1.0596.
(2) Obtained by distillation of Tuimazin crude between 440 and 520 °C; stocks obtained by division of oil fraction on silica gel by liquid chromatography.

**Estimated Error:**
Not specified.

**References:**
[1]S. V. Bondarev and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 10 (1968).

## 3.64. Paraffins

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Paraffins

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (8), 26–8 (1968).

**Variables:**
$T$/K= 258–325

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

### Experimental Data

The solubilities of paraffins (2) in nitroethane (1) over the indicated temperature range were presented in a graph as plots of temperature against log solubility. The data in the table below were extracted compilers from the reported graphs.

Solubility of paraffins (2) in nitroethane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| | | Paraffin* | | |
| −15.7 | 257.5 | 0.04 | 0.04 | 0.0001 |
| −14.0 | 259.2 | 0.08 | 0.08 | 0.0003 |
| −10.4 | 262.8 | 0.11 | 0.11 | 0.0004 |
| 0.0 | 273.2 | 0.3 | 0.3 | 0.0010 |
| 7.9 | 281.1 | 0.7 | 0.7 | 0.0024 |
| 12.1 | 285.3 | 1.0 | 1.0 | 0.0035 |
| | | Paraffin** | | |
| 6.9 | 280.1 | 0.07 | 0.07 | 0.0002 |
| 10.6 | 283.8 | 0.1 | 0.1 | 0.0003 |
| 17.6 | 290.8 | 0.3 | 0.3 | 0.0009 |
| 21.4 | 294.6 | 0.5 | 0.5 | 0.0015 |
| 25.4 | 298.6 | 0.7 | 0.7 | 0.0021 |
| 28.0 | 301.2 | 1.0 | 1.0 | 0.0030 |
| | | Paraffin*** | | |
| 17.0 | 290.2 | 0.05 | 0.05 | 0.0001 |
| 20.0 | 293.2 | 0.07 | 0.07 | 0.0002 |
| 26.5 | 299.7 | 0.17 | 0.17 | 0.0004 |
| 30.0 | 303.2 | 0.3 | 0.3 | 0.0007 |
| 34.9 | 308.1 | 0.6 | 0.6 | 0.0015 |
| 37.6 | 310.8 | 0.7 | 0.7 | 0.0018 |
| 40.0 | 313.2 | 1.2 | 1.2 | 0.0030 |
| | | Paraffin**** | | |
| 25.7 | 298.9 | 0.05 | 0.05 | 0.0001 |
| 31.1 | 304.3 | 0.08 | 0.08 | 0.0002 |
| 33.7 | 306.9 | 0.1 | 0.1 | 0.0002 |
| 42.9 | 316.1 | 0.3 | 0.3 | 0.0007 |
| 46.7 | 319.9 | 0.5 | 0.5 | 0.0011 |
| 48.5 | 321.7 | 0.7 | 0.7 | 0.0016 |
| 51.3 | 324.5 | 1.0 | 1.0 | 0.0022 |

NOTE: Footnotes explained in Source and Purity of Materials section, below.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) * and ** obtained by separation of narrow fraction with boiling point*=196 °C–270 °C and boiling point**=300 °C–365 °C from a wide fraction of diesel fuel; melting point*=13.2 °C and melting point**=28.0 °C; *** and **** obtained by separation of the third oil fraction of Tuimazin crude; melting point***=41.7 °C and melting point****=50.7 °C.

**Estimated Error:**
Not reported.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 3.65. Uranium bis (nitrato-O) dioxohexahydrate

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Uranium bis (nitrato-O) dioxohexahydrate; $UO_2(NO_3)_2 \cdot 6H_2O$; [13520-83-7]

**Original Measurements:**
R. K. Warner, Austral. J. Appl. Sci. **4**, 581–9 (1953).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

### Experimental Data

The solubility of uranyl nitrate (2) in nitroethane (1) at 293 K was reported to be 100 $w_2$ = 5.1. The corresponding mole fraction, $x_2$, calculated by the compiler is 0.010.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The analytical method was used. (2) was placed with the appropriate amount of pure (1) in small flask. The contents of the flask were warmed to 30 °C–50 °C, agitated with excess (2) for 15 min, and then placed in a constant temperature bath at 20 °C with intermittent shaking for 6–8 h. Crystallization from the supersaturated solution occurred, and when equilibrium was reached the solution was quickly decanted, filtered to remove the fine crystals, and placed in a stoppered flask at 20 °C before analysis.

**Source and Purity of Materials:**
(1) Synthesized by standard method; thoroughly dried and fractionally distilled.
(2) Source not specified; A. R. grade; not purified.

**Estimated Error:**
Temperature: ±0.05 K,
Solubility: ±0.2 g/100 g solution.

# 4. Ternary Systems Nitroethane+Water+Organic Compound

## 4.1. 2-Propenamide

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 2-Propenamide; $C_3H_5NO$; [79-06-1]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
K. Duraiswamy and G. W. Minard, J. Chem. Eng. Data **18**, 203–5 (1973).

**Variables:**
$T$/K = 292–303

**Prepared By:**
V. P. Sazonov and N. I. Lisov

### Experimental Data

The distribution of 2-propenamide (2) between coexisting liquid phases system nitroethane (1)+2-propenamide (2)+water (3)

| $t$/°C | $T$/K (compilers) | Water-rich phase 100 $w_2''$ | Nitroethane-rich phase 100 $w_2'$ | $K_2$, distribution coefficient[a] | B, selectivity[b] |
|---|---|---|---|---|---|
| 18.5 | 291.7 | 1.38 | 0.37 | 0.27 | 22.80 |
| | | 4.90 | 0.48 | 0.098 | 6.72 |
| | | 9.22 | 0.97 | 0.11 | 8.38 |
| | | 12.20 | 1.26 | 0.10 | 8.70 |
| | | 18.05 | 1.56 | 0.09 | 6.64 |
| | | 26.78 | 3.20 | 0.12 | 3.90 |
| | | 34.12 | 4.24 | 0.13 | 2.64 |
| 25.0 | 298.2 | 1.30 | 0.26 | 0.20 | 14.90 |
| | | 4.00 | 0.74 | 0.15 | 10.80 |
| | | 10.09 | 0.82 | 0.08 | 4.94 |
| | | 13.48 | 1.64 | 0.12 | 7.20 |
| | | 20.08 | 2.98 | 0.15 | 5.89 |
| 30.0 | 303.2 | 1.01 | 0.19 | 0.19 | 14.70 |
| | | 4.90 | 0.65 | 0.13 | 10.40 |
| | | 9.56 | 1.42 | 0.15 | 8.50 |
| | | 13.14 | 1.69 | 0.13 | 6.83 |
| | | 17.88 | 2.23 | 0.12 | 4.14 |
| | | 26.72 | 4.10 | 0.15 | 2.85 |
| | | 38.37 | 7.07 | 0.18 | 1.75 |
| | | 45.49 | 10.38 | 0.23 | 1.26 |

[a] $K_2 = w_2'/w_2''$, distribution coefficient is the ratio of concentration of a component (2) in coexistence liquid phases.
[b] $B = K_3/K_2$, selectivity is the ratio of distribution coefficients of two components.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The cloud-point[1] and analytical methods were used. The liquid/liquid equilibrium curve was determined by the former, and compositions of equilibrium liquid phases by the latter. The three components, in such amounts as to form two liquid phases, were added to a separatory funnel, shaken while immersed at constant temperature for 4–5 h, and allowed to settle into two layers. The two layers were separated and kept at constant temperature while the density of each was measured. Samples of each layer were analyzed for (2) content. Since these compositions must lie on the binodal curve, complete equilibrium compositions of the conjugate phases were known.

**Source and Purity of Materials:**
(1) Source not specified; commercial reagent grade; not purified.
(2) Eastman Kodak White grade; not purified.
(3) Not specified.

**Estimated Error:**
Temperature: ±0.5 K, weighing: to 0.1 mg, titer: ±0.05 mL.

**References:**
[1] R. E. Treybal, *Liquid Extraction* (McGraw–Hill, New York, 1963).

## 4.2. 2-Propanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2-Propanol; $C_3H_8O$; [67-63-0]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
T. S. Tolstova and T. V. Sheblom, Sb. Nauch. Tr., Gos. Inst. Prikl. Khim. (Leningrad) 20–3 (1975).

**Variables:**
$T$/K = 293

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Table 1. Mutual solubility of nitroethane (1), 2-propanol (2) and water (3)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 20.0 | 293.2 | 4.5 | 0.00 | 0.011 | 0.000 |
| | | 4.2 | 10.0 | 0.011 | 0.033 |
| | | 5.0 | 15.0 | 0.014 | 0.053 |
| | | 6.0 | 20.0 | 0.018 | 0.074 |
| | | 9.0 | 25.0 | 0.029 | 0.099 |
| | | 14.0 | 30.0 | 0.049 | 0.132 |
| | | 25.0 | 34.0 | 0.105 | 0.178 |
| | | 38.0 | 34.0 | 0.193 | 0.216 |
| | | 53.0 | 30.0 | 0.329 | 0.232 |
| | | 64.7 | 25.0 | 0.466 | 0.225 |
| | | 73.0 | 20.0 | 0.574 | 0.197 |
| | | 80.5 | 15.0 | 0.682 | 0.159 |
| | | 86.8 | 10.0 | 0.771 | 0.111 |
| | | 98.5 | 0.00 | 0.941 | 0.000 |

Table 2. Composition of equilibrium liquid phases

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) | | Water-rich phase (compilers) | | Nitroethane-rich phase | | Water-rich phase | |
|---|---|---|---|---|---|---|---|---|---|
| | | $x'_1$ | $x'_2$ | $x''_1$ | $x''_2$ | 100 $w'_1$ | 100 $w'_2$ | 100 $w''_1$ | 100 $w''_2$ |
| 20.0 | 293.2 | 0.867 | 0.052 | 0.011 | 0.026 | 93.4 | 4.5 | 4.2 | 7.8 |
| | | 0.849 | 0.063 | 0.011 | 0.030 | 92.2 | 5.5 | 4.2 | 9.1 |
| | | 0.838 | 0.075 | 0.011 | 0.036 | 91.2 | 6.5 | 4.2 | 10.8 |
| | | 0.788 | 0.101 | 0.013 | 0.052 | 88.0 | 9.0 | 4.6 | 14.9 |
| | | 0.749 | 0.123 | 0.015 | 0.066 | 85.3 | 11.2 | 5.3 | 18.3 |
| | | 0.724 | 0.134 | 0.018 | 0.074 | 84.5 | 12.5 | 6.0 | 20.0 |
| | | 0.701 | 0.146 | 0.021 | 0.082 | 82.0 | 13.7 | 6.8 | 21.8 |
| | | 0.655 | 0.172 | 0.027 | 0.096 | 78.5 | 16.5 | 8.6 | 24.5 |
| | | 0.578 | 0.195 | 0.041 | 0.121 | 73.3 | 19.8 | 12.0 | 28.5 |
| | | 0.537 | 0.208 | 0.050 | 0.137 | 70.2 | 21.8 | 14.0 | 31.0 |
| | | 0.447 | 0.228 | 0.087 | 0.158 | 63.2 | 25.8 | 22.0 | 32.0 |

Estimated plait point: 100 $w_1$ = 40.7, 100 $w_2$ = 32.3 ($x_1$ = 0.210, $x_2$ = 0.209, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Two methods were used. The solubility curve was determined by the titration method. The mixtures of (1) and (3) and of (1) and (2) were titrated by the third component at thorough mixing until the appearance of weak turbidity. The compositions of equilibrium liquid phases were determined by the analytical method with the apparatus described in Tolstova and Sheblom.[1] Mixtures were thoroughly mixed with a magnetic stirrer for 2–2.5 h. After separation samples of upper and lower liquid phases were analyzed by chromatography (see Tables 1 and 2).

**Source and Purity of Materials:**
(1) Source not specified; purified by distillation through a column of 20 theoretical plates.
(2) Source not specified; purified by distillation through a column of 20 theoretical plates.
(3) Distilled.

**Estimated Error:**
Not specified.

**References:**
[1]T. S. Tolstova and T. V. Sheblom, Zh. Prikl. Khim. (Leningrad) **37**, 1771 (1975).

## 4.3. 1-Propanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Propanol; $C_3H_8O$; [71-23-8]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
J. M. Malone and R. W. Vining, J. Chem. Eng. Data **12**, 387–9 (1967).

**Variables:**
$T$/K = 298

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Table 1. Mutual solubility of nitroethane (1), 1-propanol (2) and water (3)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 25 | 298 | 5.05 | 0.00 | 0.0126 | 0.0000 |
| | | 4.83 | 3.92 | 0.0124 | 0.0126 |
| | | 4.80 | 7.68 | 0.0127 | 0.0253 |
| | | 5.23 | 11.70 | 0.0143 | 0.0399 |
| | | 5.58 | 15.63 | 0.0158 | 0.0553 |
| | | 7.48 | 19.46 | 0.0223 | 0.0723 |
| | | 9.98 | 22.93 | 0.0314 | 0.0900 |
| | | 12.50 | 25.84 | 0.0414 | 0.1070 |
| | | 15.60 | 29.39 | 0.0554 | 0.1304 |
| | | 18.65 | 31.96 | 0.0706 | 0.1510 |
| | | 22.20 | 34.58 | 0.0904 | 0.1760 |
| | | 25.91 | 36.47 | 0.1135 | 0.1996 |
| | | 32.60 | 37.50 | 0.1598 | 0.2296 |
| | | 39.49 | 36.83 | 0.2145 | 0.2498 |
| | | 46.35 | 35.06 | 0.2766 | 0.2613 |
| | | 51.92 | 32.66 | 0.3308 | 0.2599 |
| | | 58.10 | 29.70 | 0.3979 | 0.2541 |
| | | 63.43 | 26.61 | 0.4591 | 0.2406 |
| | | 69.31 | 22.94 | 0.5321 | 0.2200 |
| | | 74.77 | 19.25 | 0.6043 | 0.1943 |
| | | 80.23 | 15.45 | 0.6827 | 0.1642 |
| | | 85.37 | 11.55 | 0.7580 | 0.1281 |
| | | 90.40 | 7.70 | 0.8376 | 0.0891 |
| | | 94.98 | 3.78 | 0.9057 | 0.0450 |
| | | 99.14 | 0.00 | 0.9651 | 0.0000 |

Table 2. Composition of equilibrium liquid phases

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) | | Water-rich phase (compilers) | | Nitroethane-rich phase | | Water-rich phase | |
|---|---|---|---|---|---|---|---|---|---|
| | | $x'_1$ | $x'_2$ | $x''_1$ | $x''_2$ | 100 $w'_1$ | 100 $w'_2$ | 100 $w''_1$ | 100 $w''_2$ |
| 25 | 298 | 0.8797 | 0.0576 | 0.0124 | 0.0161 | 93.50 | 4.90 | 4.80 | 5.00 |
| | | 0.7661 | 0.1260 | 0.0134 | 0.0329 | 85.80 | 11.30 | 5.00 | 9.80 |
| | | 0.6024 | 0.1957 | 0.0143 | 0.0426 | 74.60 | 19.40 | 5.20 | 12.40 |
| | | 0.4141 | 0.2478 | 0.0157 | 0.0516 | 59.70 | 28.60 | 5.60 | 14.70 |
| | | 0.2324 | 0.2533 | 0.0202 | 0.0661 | 41.60 | 36.30 | 6.90 | 18.10 |
| | | 0.1535 | 0.2274 | 0.0292 | 0.0856 | 31.70 | 37.60 | 9.40 | 22.10 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Two methods were used. The solubility curve was determined by the titration method. A measured amount of (1) was added to a tarred 50 mL Erlenmeyer flack and titrated to the cloud point with (3). To each succeeding sample of (1) a measured quantity of (2) was added and the mixture was titrated with (3). Weight measurements were made using an analytical balance. Titrations were performed using 5 mL certified microburettes graduated in 0.01 mL divisions. The analytical method was used for determination of equilibrium liquid phases compositions. The mixture of (1), (2), and (3) was then agitated vigorously and allowed to separate into phases. Densities were used to determine compositions of the equilibrium phases. Refractive index readings were used primarily to identify phases and secondarily to check compositions from density measurements (see Tables 1 and 2).

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 93.9 mass % with 2.3 mass % of nitromethane and 3.8 mass % of 2-nitropropane; $n$(25 °C,D) = 1.3890.
(2) Fisher; certified reagent grade; boiling point = 97.0–97.4 °C, $n$(25°C,D) = 1.3871.
(3) Distilled.

**Estimated Error:**
Temperature: ±1 K.

## 4.4. 1-Nonanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976); Deposited Doc., VINITI. 1951 (1976).

**Variables:**
$T$/K=266–448

**Prepared By:**
V. P. Sazonov, N. I. Lisov, and N. V. Sazonov

**Experimental Data**

The solubility temperatures of the liquid phases were determined in ternary mixtures with a constant mass relationship of (1) and (2) as 10.0:90.0, 20.0:80.0, 30.0:70,0, 40.0:60.0, 50.0:50.0, 60.0:40.0, 70.0:30.0, 80.0:20.0 and 90.0:10.0 respectively, and also in ternary mixtures with a constant mass content of (3), respectively 20.0, 30.0, 40.0, and 50.0 (see Tables 1–3).

Table 1. Solubility temperatures of three liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass content of water=20.0 | | | |
| 2.0 | 275.2 | 30.00 | 50.00 | 0.2153 | 0.1867 |
| 2.0 | 275.2 | 60.00 | 20.00 | 0.3903 | 0.0677 |
| 3.3 | 276.5 | 35.00 | 45.00 | 0.2469 | 0.1652 |
| 3.5 | 276.7 | 55.00 | 25.00 | 0.3634 | 0.0860 |
| 4.0 | 277.2 | 40.00 | 40.00 | 0.2775 | 0.1444 |
| 4.0 | 277.2 | 45.00 | 35.00 | 0.3071 | 0.1243 |
| 4.0 | 277.2 | 50.00 | 30.00 | 0.3357 | 0.1048 |
| | | constant mass content of water=30.0 | | | |
| 0.7 | 273.9 | 55.00 | 15.00 | 0.2929 | 0.0416 |
| 2.5 | 275.7 | 25.00 | 45.00 | 0.1442 | 0.1351 |
| 2.5 | 275.7 | 50.00 | 20.00 | 0.2697 | 0.0561 |
| 3.5 | 276.7 | 45.00 | 25.00 | 0.2459 | 0.0711 |
| 3.7 | 276.9 | 30.00 | 40.00 | 0.1707 | 0.1184 |
| 4.0 | 277.2 | 35.00 | 35.00 | 0.1964 | 0.1022 |
| 4.0 | 277.2 | 40.00 | 30.00 | 0.2215 | 0.0864 |
| | | constant mass content of water=40.0 | | | |
| 0.0 | 273.2 | 20.00 | 40.00 | 0.0964 | 0.1003 |
| 2.5 | 275.7 | 45.00 | 15.00 | 0.2051 | 0.0356 |
| 3.0 | 276.2 | 25.00 | 35.00 | 0.1191 | 0.0868 |
| 3.7 | 276.9 | 40.00 | 20.00 | 0.1843 | 0.0480 |
| 4.0 | 277.2 | 30.00 | 30.00 | 0.1413 | 0.0736 |
| 4.0 | 277.2 | 35.00 | 25.00 | 0.1631 | 0.0606 |
| | | constant mass content of water=50.0 | | | |
| 1.0 | 274.2 | 40.00 | 10.00 | 0.1578 | 0.0205 |
| 2.5 | 275.7 | 20.00 | 30.00 | 0.0820 | 0.0640 |
| 3.3 | 276.5 | 35.00 | 15.00 | 0.1394 | 0.0311 |
| 4.0 | 277.2 | 25.00 | 25.00 | 0.1015 | 0.0528 |
| 4.0 | 277.2 | 30.00 | 20.00 | 0.1206 | 0.0418 |

Table 2. Solubility temperatures of two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass relationship nitroethane:1-nonanol=90.0:10.0 | | | |
| 9.0 | 282.2 | 89.46 | 9.94 | 0.9210 | 0.0533 |
| 21.5 | 294.7 | 88.92 | 9.88 | 0.8976 | 0.0519 |
| 40.0 | 313.2 | 88.56 | 9.84 | 0.8825 | 0.0510 |
| 51.0 | 324.2 | 88.20 | 9.80 | 0.8678 | 0.0502 |
| | | constant mass relationship nitroethane:1-nonanol=80.0:20.0 | | | |
| 1.5 | 274.7 | 79.20 | 19.80 | 0.8455 | 0.1100 |
| 2.5 | 275.7 | 78.88 | 19.72 | 0.8305 | 0.1080 |
| 3.3 | 276.5 | 79.52 | 19.88 | 0.8609 | 0.1120 |
| 15.0 | 288.2 | 78.56 | 19.64 | 0.8160 | 0.1062 |
| 31.5 | 304.7 | 78.32 | 19.58 | 0.8053 | 0.1048 |
| 42.0 | 315.2 | 77.92 | 19.48 | 0.7880 | 0.1025 |
| 47.0 | 320.2 | 77.76 | 19.44 | 0.7812 | 0.1016 |
| | | constant mass relationship nitroethane:1-nonanol=70.0:30.0 | | | |
| 4.5 | 277.7 | 69.02 | 29.58 | 0.7648 | 0.1706 |
| 4.5 | 277.7 | 68.88 | 29.52 | 0.7577 | 0.1690 |
| 5.0 | 278.2 | 68.67 | 29.43 | 0.7472 | 0.1666 |
| 7.0 | 280.2 | 69.58 | 29.82 | 0.7943 | 0.1771 |
| 7.5 | 280.7 | 69.65 | 29.85 | 0.7981 | 0.1780 |
| 36.0 | 309.2 | 68.46 | 29.34 | 0.7370 | 0.1644 |
| 50.0 | 323.2 | 68.25 | 29.25 | 0.7269 | 0.1621 |
| 95.0 | 368.2 | 0.0350 | 0.0150 | $8.4\cdot10^{-5}$ | $1.87\cdot10^{-5}$ |
| 105.0 | 378.2 | 0.0385 | 0.0165 | $9.25\cdot10^{-5}$ | $2.06\cdot10^{-5}$ |
| 115.0 | 388.2 | 0.0448 | 0.0192 | $1.08\cdot10^{-4}$ | $2.40\cdot10^{-5}$ |
| | | constant mass relationship nitroethane:1-nonanol=60.0:40.0 | | | |
| 4.5 | 277.7 | 58.56 | 39.04 | 0.6589 | 0.2286 |
| 5.0 | 278.2 | 58.92 | 39.28 | 0.6783 | 0.2353 |
| 5.5 | 278.7 | 59.16 | 39.44 | 0.6918 | 0.2400 |
| 6.5 | 279.7 | 59.34 | 39.56 | 0.7022 | 0.2436 |
| 7.0 | 280.2 | 59.46 | 39.64 | 0.7092 | 0.2460 |
| 8.6 | 281.8 | 59.70 | 39.80 | 0.7237 | 0.2511 |
| 9.5 | 282.7 | 59.88 | 39.92 | 0.7348 | 0.2549 |
| 9.5 | 282.7 | 58.44 | 38.96 | 0.6526 | 0.2264 |
| 23.5 | 296.7 | 58.20 | 38.80 | 0.6403 | 0.2221 |
| 36.0 | 309.2 | 57.96 | 38.64 | 0.6284 | 0.2180 |
| 49.0 | 322.2 | 57.60 | 38.40 | 0.6112 | 0.2120 |
| | | constant mass relationship nitroethane:1-nonanol=50.0:50.0 | | | |
| 4.5 | 277.7 | 48.80 | 48.80 | 0.5796 | 0.3016 |
| 4.5 | 277.7 | 48.60 | 48.60 | 0.5681 | 0.2956 |
| 5.0 | 278.2 | 48.85 | 48.85 | 0.5826 | 0.3032 |
| 5.5 | 278.7 | 49.10 | 49.10 | 0.5977 | 0.3110 |
| 6.0 | 279.2 | 49.30 | 49.30 | 0.6102 | 0.3176 |
| 7.5 | 280.7 | 49.55 | 49.55 | 0.6265 | 0.3260 |
| 9.0 | 282.2 | 49.80 | 49.80 | 0.6436 | 0.3349 |
| 20.0 | 293.2 | 48.40 | 48.40 | 0.5569 | 0.2898 |
| 33.5 | 306.7 | 48.25 | 48.25 | 0.5487 | 0.2855 |
| 40.0 | 313.2 | 48.20 | 48.20 | 0.5460 | 0.2841 |
| 94.0 | 367.2 | 0.0265 | 0.0265 | $6.36\cdot10^{-5}$ | $3.31\cdot10^{-5}$ |
| 113.0 | 386.2 | 0.0290 | 0.0290 | $6.96\cdot10^{-5}$ | $3.62\cdot10^{-5}$ |
| 125.0 | 398.2 | 0.0315 | 0.0315 | $7.57\cdot10^{-5}$ | $3.94\cdot10^{-5}$ |
| | | constant mass relationship nitroethane:1-nonanol=40.0:60.0 | | | |

| | | | | | |
|---|---|---|---|---|---|
| 3.5 | 276.7 | 38.80 | 58.20 | 0.4756 | 0.3712 |
| 3.5 | 276.7 | 38.64 | 57.96 | 0.4657 | 0.3635 |
| 4.0 | 277.2 | 38.96 | 58.44 | 0.4858 | 0.3792 |
| 4.5 | 277.7 | 39.08 | 58.62 | 0.4936 | 0.3853 |
| 5.0 | 278.2 | 39.24 | 58.86 | 0.5045 | 0.3938 |
| 6.0 | 279.2 | 39.48 | 59.22 | 0.5214 | 0.4070 |
| 7.0 | 280.2 | 39.60 | 59.40 | 0.5303 | 0.4139 |
| 8.0 | 281.2 | 39.76 | 59.64 | 0.5425 | 0.4234 |
| 18.0 | 291.2 | 38.48 | 57.72 | 0.4562 | 0.3561 |
| 27.5 | 300.7 | 38.36 | 57.54 | 0.4493 | 0.3507 |
| 40.0 | 313.2 | 38.20 | 57.30 | 0.4403 | 0.3437 |
| constant mass relationship nitroethane:1-nonanol=30.0:70.0 | | | | | |
| 0.0 | 273.2 | 29.04 | 67.76 | 0.3741 | 0.4542 |
| 0.0 | 273.2 | 29.01 | 67.69 | 0.3720 | 0.4517 |
| 0.5 | 273.7 | 28.89 | 67.41 | 0.3639 | 0.4419 |
| 1.0 | 274.2 | 29.10 | 67.90 | 0.3783 | 0.4593 |
| 2.0 | 275.2 | 29.34 | 68.46 | 0.3958 | 0.4806 |
| 3.0 | 276.2 | 29.49 | 68.81 | 0.4074 | 0.4947 |
| 4.0 | 277.2 | 29.70 | 69.30 | 0.4247 | 0.5157 |
| 5.5 | 278.7 | 29.85 | 69.65 | 0.4378 | 0.5316 |
| 11.0 | 284.2 | 28.74 | 67.06 | 0.3542 | 0.4301 |
| 41.0 | 314.2 | 28.50 | 66.50 | 0.3395 | 0.4123 |
| 100.0 | 373.2 | 0.0168 | 0.0392 | $4.03\cdot10^{-5}$ | $4.90\cdot10^{-5}$ |
| 120.0 | 393.2 | 0.0180 | 0.0420 | $4.32\cdot10^{-5}$ | $5.24\cdot10^{-5}$ |
| 140.0 | 413.2 | 0.0192 | 0.0448 | $4.61\cdot10^{-5}$ | $5.60\cdot10^{-5}$ |
| constant mass relationship nitroethane:1-nonanol=20.0:80.0 | | | | | |
| −7.0 | 266.2 | 19.28 | 77.12 | 0.2591 | 0.5393 |
| −7.0 | 266.2 | 19.20 | 76.80 | 0.2532 | 0.5270 |
| −6.5 | 266.7 | 19.38 | 77.52 | 0.2668 | 0.5554 |
| −6.0 | 267.2 | 19.54 | 78.16 | 0.2800 | 0.5828 |
| −5.5 | 267.7 | 19.62 | 78.48 | 0.2869 | 0.5973 |
| −4.0 | 269.2 | 19.74 | 78.96 | 0.2980 | 0.6203 |
| −1.5 | 271.7 | 19.90 | 79.60 | 0.3139 | 0.6533 |
| 17.0 | 290.2 | 19.10 | 76.40 | 0.2461 | 0.5123 |
| 44.0 | 317.2 | 19.04 | 76.16 | 0.2420 | 0.5038 |
| constant mass relationship nitroethane:1-nonanol=10.0:90.0 | | | | | |
| −4.0 | 269.2 | 9.74 | 87.66 | 0.1472 | 0.6812 |
| 4.0 | 277.2 | 9.70 | 87.30 | 0.1434 | 0.6718 |
| 20.0 | 293.2 | 9.65 | 86.85 | 0.1390 | 0.6510 |
| 36.0 | 309.2 | 9.59 | 86.31 | 0.1340 | 0.6274 |
| constant mass content of water=45.0 | | | | | |
| 168.5 | 441.7 | 54.50 | 0.50 | 0.2250 | 0.0011 |
| 169.5 | 442.7 | 54.80 | 0.20 | 0.2261 | 0.0004 |
| 169.5 | 442.7 | 53.90 | 1.10 | 0.2228 | 0.0024 |
| 170.0 | 443.2 | 55.00 | ⋯ | 0.2268 | ⋯ |
| 172.0 | 445.2 | 53.00 | 2.00 | 0.2195 | 0.0043 |
| 174.0 | 447.2 | 51.00 | 4.00 | 0.2120 | 0.0087 |
| 175.0 | 448.2 | 50.00 | 5.00 | 0.2083 | 0.0108 |

Table 3. Compositions of two and three coexisting liquid phases system nitroethane+1-nonanol+water*

| | | Nitroethane-rich phase | | Alcohol-rich phase | | Water-rich phase | |
|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $100\ w_1'$ | $100\ w_2'$ | $100\ w_1''$ | $100\ w_2''$ | $100\ w_1'''$ | $100\ w_2'''$ |
| 0.0 | 273.2 | 81.2 | 16.8 | 31.5 | 64.9 | 4.2 | 0.3 |
| | | 88.2 | 10.2 | ⋯ | ⋯ | 4.1 | 0.2 |
| | | 93.4 | 5.9 | ⋯ | ⋯ | 4.0 | 0.1 |
| | | ⋯ | ⋯ | 29.0 | 67.0 | 3.2 | 0.2 |
| | | ⋯ | ⋯ | 21.2 | 74.7 | 2.3 | 0.2 |
| | | ⋯ | ⋯ | 12.6 | 83.3 | 1.4 | 0.1 |
| | | ⋯ | ⋯ | 6.0 | 89.8 | 0.7 | 0.1 |
| 4.0 | 277.2 | 60.6 | 36.4 | 46.5 | 49.6 | 4.3 | 0.3 |
| | | 67.0 | 31.3 | ⋯ | ⋯ | 4.2 | 0.3 |
| | | 73.0 | 25.8 | ⋯ | ⋯ | 4.1 | 0.2 |
| | | 80.0 | 18.9 | ⋯ | ⋯ | 4.2 | 0.2 |
| | | 88.0 | 12.4 | ⋯ | ⋯ | 4.2 | 0.1 |
| | | 94.1 | 5.7 | ⋯ | ⋯ | 4.3 | 0.1 |
| | | ⋯ | ⋯ | 37.2 | 58.8 | 3.3 | 0.2 |
| | | ⋯ | ⋯ | 25.4 | 70.5 | 2.4 | 0.2 |
| | | ⋯ | ⋯ | 17.3 | 78.5 | 1.6 | 0.1 |
| | | ⋯ | ⋯ | 9.0 | 86.7 | 0.8 | 0.1 |

The same data are presented below in mole fractions

| | | Nitroethane-rich phase (compilers) | | Alcohol-rich phase (compilers) | | Water-rich phase (compilers) | |
|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ | $x_1'''$ | $x_2'''$ |
| 0.0 | 273.2 | 0.826 | 0.089 | 0.392 | 0.421 | 0.0104 | 0.0004 |
| | | 0.881 | 0.053 | ⋯ | ⋯ | 0.0102 | 0.0003 |
| | | 0.940 | 0.031 | ⋯ | ⋯ | 0.0099 | 0.0001 |
| | | ⋯ | ⋯ | 0.360 | 0.433 | 0.0079 | 0.0003 |
| | | ⋯ | ⋯ | 0.275 | 0.504 | 0.0056 | 0.0001 |
| | | ⋯ | ⋯ | 0.172 | 0.594 | 0.0034 | 0.0001 |
| | | ⋯ | ⋯ | 0.085 | 0.666 | 0.0017 | 0.0001 |
| 4.0 | 277.2 | 0.658 | 0.206 | 0.525 | 0.292 | 0.0107 | 0.0004 |
| | | 0.741 | 0.180 | ⋯ | ⋯ | 0.0104 | 0.0004 |
| | | 0.799 | 0.147 | ⋯ | ⋯ | 0.0102 | 0.0003 |
| | | 0.847 | 0.104 | ⋯ | ⋯ | 0.0104 | 0.0003 |
| | | 0.948 | 0.070 | ⋯ | ⋯ | 0.0104 | 0.0001 |
| | | 0.961 | 0.030 | ⋯ | ⋯ | 0.0107 | 0.0001 |
| | | ⋯ | ⋯ | 0.440 | 0.362 | 0.0081 | 0.0004 |
| | | ⋯ | ⋯ | 0.321 | 0.463 | 0.0059 | 0.0003 |
| | | ⋯ | ⋯ | 0.229 | 0.540 | 0.0039 | 0.0001 |
| | | ⋯ | ⋯ | 0.125 | 0.626 | 0.0019 | 0.0001 |

*The compilers extracted these data from the published graphs.

## Auxiliary Information

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures of the liquid phase were determined by the synthetic method.[1] The analytical method described in Nikurashina and Mertslin[2] was used for determining equilibrium liquid phase compositions. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; purity not specified; distilled; $n(20\ °C,D)=1.3905$, $d(20\ °C,4\ °C)=1.0525$.
(2) Source not specified, purity not specified; distilled; $n(20\ °C,D)=1.4300$, $d(20\ °C,4\ °C)=0.8270$.
(3) $n(20\ °C,D)=1.333$.

**Estimated Error:**

Not specified.

**References:**

[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).
[2]N. I. Nikurashina and R. V. Mertslin, *Method of Secants* (in Russian) (Saratov University Press, 1969).

## 4.5. 1-Decanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
I. K. Zhuravleva, E. F. Zhuravlev, and T. L. Khotkovskaya, Zh. Prikl. Khim. (Leningrad) **49**, 2586 (1976); Deposited Doc., VINITI. 1951 (1976).

**Variables:**
$T$/K=270–454

**Prepared By:**
V. P. Sazonov, N. I. Lisov, and N. V. Sazonov

**Experimental Data**

The solubility temperatures of the liquid phases were determined in ternary mixtures with a constant mass content of (3), respectively 20.0, 30.0, 45.0, and 60.0 mass % and in ternary mixtures with constant mass relationship of (1) and (2) as 10.0:90.0, 20.0:80.0, 30.0:70,0, 40.0:60.0, 50.0:50.0, 60.0:40.0, 70.0:30.0, 80.0:20.0, and 90.0:10.0, respectively (see Tables 1–3).

Table 1. Solubility temperatures of three liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass content of water=20.0 | | | |
| 12.0 | 285.2 | 30.0 | 50.0 | 0.219 | 0.173 |
| 13.5 | 286.7 | 60.0 | 20.0 | 0.393 | 0.062 |
| 14.5 | 287.7 | 35.0 | 45.0 | 0.251 | 0.153 |
| 15.0 | 288.2 | 55.0 | 25.0 | 0.366 | 0.079 |
| 16.0 | 289.2 | 40.0 | 40.0 | 0.281 | 0.133 |
| 16.0 | 289.2 | 45.0 | 35.0 | 0.311 | 0.114 |
| 16.0 | 289.2 | 50.0 | 30.0 | 0.339 | 0.096 |
| | | constant mass content of water=30.0 | | | |
| 11.5 | 284.7 | 25.0 | 45.0 | 0.146 | 0.125 |
| 12.5 | 285.7 | 55.0 | 15.0 | 0.294 | 0.038 |
| 14.5 | 287.7 | 30.0 | 40.0 | 0.172 | 0.109 |
| 14.5 | 287.7 | 50.0 | 20.0 | 0.271 | 0.051 |
| 16.0 | 289.2 | 35.0 | 35.0 | 0.198 | 0.094 |
| 16.0 | 289.2 | 40.0 | 30.0 | 0.223 | 0.079 |
| 16.0 | 289.2 | 45.0 | 25.0 | 0.247 | 0.065 |
| | | constant mass content of water=45.0 | | | |
| 10.0 | 283.2 | 45.0 | 10.0 | 0.190 | 0.020 |
| 11.0 | 284.2 | 20.0 | 35.0 | 0.089 | 0.071 |
| 14.0 | 287.2 | 40.0 | 15.0 | 0.170 | 0.030 |
| 15.5 | 288.7 | 25.0 | 30.0 | 0.110 | 0.063 |
| 16.0 | 289.2 | 30.0 | 25.0 | 0.131 | 0.052 |
| 16.0 | 289.2 | 35.0 | 20.0 | 0.151 | 0.041 |
| | | constant mass content of water=60.0 | | | |
| 10.5 | 283.7 | 32.5 | 7.5 | 0.114 | 0.012 |
| 12.0 | 285.2 | 15.0 | 25.0 | 0.054 | 0.043 |
| 13.0 | 286.2 | 30.0 | 10.0 | 0.105 | 0.017 |
| 14.0 | 287.2 | 27.5 | 12.5 | 0.097 | 0.021 |
| 14.5 | 287.7 | 17.5 | 22.5 | 0.063 | 0.038 |
| 15.5 | 288.7 | 20.0 | 20.0 | 0.072 | 0.034 |
| 15.5 | 288.7 | 25.0 | 15.0 | 0.089 | 0.025 |
| 16.0 | 289.2 | 22.5 | 17.5 | 0.080 | 0.030 |

Table 2. Solubility temperatures of two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass relationship nitroethane:1-decanol=90.0:10.0 | | | |
| 2.5 | 275.7 | 89.2 | 9.9 | 0.914 | 0.048 |
| 3.0 | 276.2 | 89.7 | 10.0 | 0.938 | 0.049 |
| 25.5 | 298.7 | 88.9 | 9.9 | 0.902 | 0.048 |
| 35.5 | 308.7 | 88.7 | 9.9 | 0.894 | 0.047 |
| 44.5 | 317.7 | 88.6 | 9.8 | 0.890 | 0.047 |
| | | constant mass relationship nitroethane:1-decanol=80.0:20.0 | | | |
| 12.5 | 285.7 | 79.2 | 19.8 | 0.854 | 0.101 |
| 14.0 | 287.2 | 79.6 | 19.9 | 0.874 | 0.103 |
| 15.5 | 288.7 | 78.9 | 19.7 | 0.839 | 0.099 |
| 38.5 | 311.7 | 78.8 | 19.7 | 0.835 | 0.099 |
| | | constant mass relationship nitroethane:1-decanol=70.0:30.0 | | | |
| 15.6 | 288.8 | 68.5 | 29.4 | 0.751 | 0.153 |
| 15.6 | 288.8 | 68.2 | 29.2 | 0.734 | 0.149 |
| 15.7 | 288.9 | 68.7 | 29.5 | 0.762 | 0.155 |
| 16.0 | 289.2 | 69.0 | 29.6 | 0.776 | 0.158 |
| 16.5 | 289.7 | 69.2 | 29.6 | 0.784 | 0.159 |
| 17.5 | 290.7 | 67.9 | 29.1 | 0.721 | 0.146 |
| 18.5 | 291.7 | 69.6 | 29.8 | 0.811 | 0.165 |
| 62.5 | 335.7 | 67.8 | 29.0 | 0.714 | 0.145 |
| 91.0 | 364.2 | 0.028 | 0.012 | $6.72\cdot10^{-5}$ | $1.37\cdot10^{-5}$ |
| 107.0 | 380.2 | 0.031 | 0.014 | $7.56\cdot10^{-5}$ | $1.93\cdot10^{-5}$ |
| 119.0 | 392.2 | 0.037 | 0.016 | $8.90\cdot10^{-5}$ | $1.81\cdot10^{-5}$ |
| 130.0 | 403.2 | 0.042 | 0.018 | 0.0001 | $2.05\cdot10^{-5}$ |
| | | constant mass relationship nitroethane:1-decanol=60.0:40.0 | | | |
| 16.0 | 289.2 | 58.8 | 39.2 | 0.686 | 0.2167 |
| 16.5 | 289.7 | 59.2 | 39.5 | 0.710 | 0.2245 |
| 17.0 | 290.2 | 59.3 | 39.6 | 0.718 | 0.2270 |
| 18.5 | 291.7 | 59.6 | 39.8 | 0.736 | 0.223 |
| 19.5 | 292.7 | 59.8 | 39.8 | 0.744 | 0.235 |
| 23.5 | 296.7 | 57.6 | 38.4 | 0.623 | 0.197 |
| 34.5 | 307.7 | 57.3 | 38.2 | 0.609 | 0.192 |
| 46.5 | 319.7 | 57.0 | 38.0 | 0.595 | 0.188 |
| | | constant mass relationship nitroethane:1-decanol=50.0:50.0 | | | |
| 16.0 | 289.2 | 48.5 | 48.5 | 0.580 | 0.275 |
| 16.5 | 289.7 | 48.9 | 48.9 | 0.605 | 0.287 |
| 17.5 | 290.7 | 49.4 | 49.4 | 0.635 | 0.301 |
| 19.0 | 292.2 | 49.6 | 49.6 | 0.649 | 0.308 |
| 24.5 | 297.7 | 48.2 | 48.2 | 0.560 | 0.266 |
| 35.0 | 308.2 | 47.7 | 47.7 | 0.536 | 0.254 |
| 48.5 | 321.7 | 47.5 | 47.5 | 0.523 | 0.248 |
| 95.0 | 368.2 | 0.0235 | 0.0235 | $5.64\cdot10^{-5}$ | $2.68\cdot10^{-5}$ |
| 113.0 | 386.2 | 0.025 | 0.025 | $6.00\cdot10^{-5}$ | $2.85\cdot10^{-5}$ |
| 128.0 | 401.2 | 0.027 | 0.027 | $6.48\cdot10^{-5}$ | $3.08\cdot10^{-5}$ |
| 144.0 | 417.2 | 0.0315 | 0.0315 | $7.56\cdot10^{-5}$ | $3.59\cdot10^{-5}$ |
| | | constant mass relationship nitroethane:1-decanol=40.0:60.0 | | | |
| 16.0 | 289.2 | 39.5 | 59.2 | 0.541 | 0.385 |
| 16.5 | 289.7 | 39.5 | 59.3 | 0.544 | 0.387 |
| 17.0 | 290.2 | 39.6 | 59.4 | 0.551 | 0.392 |
| 17.5 | 290.7 | 39.6 | 59.4 | 0.554 | 0.394 |
| 18.5 | 291.7 | 39.7 | 59.5 | 0.557 | 0.396 |

| | | | | | |
|---|---|---|---|---|---|
| 19.0 | 292.2 | 39.8 | 59.7 | 0.567 | 0.403 |
| 27.5 | 300.7 | 39.0 | 58.4 | 0.503 | 0.358 |
| 42.5 | 315.7 | 38.8 | 58.2 | 0.492 | 0.350 |
| constant mass relationship nitroethane:1-decanol=30.0:70.0 | | | | | |
| 12.0 | 285.2 | 29.5 | 68.8 | 0.426 | 0.472 |
| 12.5 | 285.7 | 29.6 | 69.1 | 0.437 | 0.483 |
| 13.5 | 286.7 | 29.7 | 69.3 | 0.445 | 0.493 |
| 15.0 | 288.2 | 29.7 | 69.4 | 0.448 | 0.496 |
| 16.0 | 289.2 | 29.8 | 69.6 | 0.457 | 0.505 |
| 26.0 | 299.2 | 29.4 | 68.6 | 0.418 | 0.463 |
| 50.5 | 323.7 | 29.3 | 68.4 | 0.411 | 0.455 |
| 102.0 | 375.2 | 0.0174 | 0.0406 | $4.18\cdot10^{-5}$ | $4.62\cdot10^{-5}$ |
| 120.0 | 393.2 | 0.018 | 0.042 | $4.32\cdot10^{-5}$ | $4.78\cdot10^{-5}$ |
| 146.0 | 419.2 | 0.0195 | 0.0455 | $4.68\cdot10^{-5}$ | $5.18\cdot10^{-5}$ |
| constant mass relationship nitroethane:1-decanol=20.0:80.0 | | | | | |
| 5.5 | 278.7 | 19.6 | 78.2 | 0.297 | 0.564 |
| 6.0 | 279.2 | 19.6 | 78.4 | 0.301 | 0.571 |
| 6.5 | 279.7 | 19.7 | 78.7 | 0.309 | 0.586 |
| 7.0 | 280.2 | 19.7 | 79.0 | 0.315 | 0.598 |
| 8.0 | 281.2 | 19.8 | 79.0 | 0.317 | 0.602 |
| 9.5 | 282.7 | 19.9 | 79.5 | 0.331 | 0.628 |
| 25.5 | 298.7 | 19.4 | 77.6 | 0.282 | 0.536 |
| 45.0 | 318.2 | 19.4 | 77.4 | 0.279 | 0.529 |
| constant mass relationship nitroethane:1-decanol=10.0:90.0 | | | | | |
| −3.5 | 269.7 | 9.9 | 89.0 | 0.175 | 0.745 |
| −3.0 | 270.2 | 9.9 | 89.4 | 0.181 | 0.773 |
| −1.0 | 272.2 | 10.0 | 89.5 | 0.183 | 0.779 |
| 0.5 | 272.7 | 9.8 | 87.8 | 0.159 | 0.679 |
| 16.0 | 289.2 | 9.7 | 87.5 | 0.155 | 0.660 |
| 49.5 | 322.7 | 9.6 | 86.4 | 0.143 | 0.609 |
| constant mass content of water=45.0 | | | | | |
| 170.0 | 443.2 | 54.5 | 0.5 | 0.225 | 0.010 |
| 170.0 | 443.2 | 54.0 | 1.0 | 0.223 | 0.020 |
| 170.5 | 443.7 | 55.0 | ⋯ | 0.227 | ⋯ |
| 173.0 | 446.2 | 53.0 | 2.0 | 0.220 | 0.004 |
| 178.0 | 451.2 | 51.0 | 4.0 | 0.212 | 0.008 |
| 181.0 | 454.2 | 49.0 | 6.0 | 0.205 | 0.012 |

Table 3. Compositions of two and three coexisting liquid phases system nitroethane+1-decanol+water*

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase | | Alcohol-rich phase | | Water-rich phase | |
|---|---|---|---|---|---|---|---|
| | | $100\ w_1'$ | $100\ w_2'$ | $100\ w_1''$ | $100\ w_2''$ | $100\ w_1'''$ | $100\ w_2'''$ |
| 14.0 | 287.2 | 73.1 | 25.2 | 38.2 | 69.0 | 4.0 | 0.2 |
| | | 76.5 | 22.3 | ⋯ | ⋯ | 3.9 | 0.2 |
| | | 85.3 | 13.8 | ⋯ | ⋯ | 3.8 | 0.1 |
| | | 90.5 | 8.9 | ⋯ | ⋯ | 3.9 | 0.1 |
| | | 96.1 | 3.7 | ⋯ | ⋯ | 4.0 | 0.1 |
| | | ⋯ | ⋯ | 31.0 | 67.0 | 3.0 | 0.2 |
| | | ⋯ | ⋯ | 24.5 | 73.0 | 2.4 | 0.1 |
| | | ⋯ | ⋯ | 17.0 | 80.0 | 1.6 | 0.1 |
| | | ⋯ | ⋯ | 11.0 | 86.0 | 0.6 | 0.1 |
| 15.5 | 288.7 | 65.3 | 32.9 | 45.3 | 52.8 | 4.1 | 0.2 |
| | | 75.6 | 22.8 | ⋯ | ⋯ | 4.0 | 0.2 |
| | | 83.4 | 15.4 | ⋯ | ⋯ | 3.9 | 0.1 |
| | | 90.1 | 9.1 | ⋯ | ⋯ | 4.0 | 0.1 |
| | | ⋯ | ⋯ | 36.9 | 60.9 | 3.1 | 0.2 |
| | | ⋯ | ⋯ | 28.7 | 68.8 | 2.4 | 0.1 |
| | | ⋯ | ⋯ | 15.8 | 81.5 | 1.6 | 0.1 |
| | | ⋯ | ⋯ | 7.3 | 89.6 | 0.7 | 0.1 |
| 16.0 | 289.2 | 62.3 | 35.8 | 47.5 | 50.5 | 4.1 | 0.2 |
| | | 68.5 | 29.8 | ⋯ | ⋯ | 4.0 | 0.2 |
| | | 72.8 | 25.7 | ⋯ | ⋯ | 4.0 | 0.1 |
| | | 79.1 | 19.6 | ⋯ | ⋯ | 3.9 | 0.1 |
| | | 84.1 | 14.8 | ⋯ | ⋯ | 4.0 | 0.1 |
| | | 89.3 | 9.8 | ⋯ | ⋯ | 4.1 | 0.1 |
| | | 95.4 | 4.3 | ⋯ | ⋯ | 4.2 | 0.1 |
| | | ⋯ | ⋯ | 41.7 | 56.2 | 3.5 | 0.2 |
| | | ⋯ | ⋯ | 35.9 | 61.9 | 2.9 | 0.2 |
| | | ⋯ | ⋯ | 28.7 | 68.9 | 2.3 | 0.1 |
| | | ⋯ | ⋯ | 22.5 | 74.9 | 1.7 | 0.1 |
| | | ⋯ | ⋯ | 15.7 | 81.5 | 1.2 | 0.1 |
| | | ⋯ | ⋯ | 7.2 | 89.4 | 0.7 | 0.1 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) | | Alcohol-rich phase (compilers) | | Water-rich phase (compilers) | |
|---|---|---|---|---|---|---|---|
| | | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ | $x_1'''$ | $x_2'''$ |
| 14.0 | 287.2 | 0.793 | 0.130 | 0.515 | 0.384 | 0.0099 | 0.0002 |
| | | 0.831 | 0.115 | ⋯ | ⋯ | 0.0097 | 0.0002 |
| | | 0.892 | 0.069 | ⋯ | ⋯ | 0.0094 | 0.0001 |
| | | 0.931 | 0.043 | ⋯ | ⋯ | 0.0097 | 0.0001 |
| | | 0.974 | 0.018 | ⋯ | ⋯ | 0.0099 | 0.0001 |
| | | ⋯ | ⋯ | 0.436 | 0.447 | 0.0074 | 0.0002 |
| | | ⋯ | ⋯ | 0.352 | 0.498 | 0.0059 | 0.0001 |
| | | ⋯ | ⋯ | 0.252 | 0.563 | 0.0039 | 0.0001 |
| | | ⋯ | ⋯ | 0.171 | 0.635 | 0.0014 | 0.0001 |
| 15.5 | 288.7 | 0.739 | 0.177 | 0.579 | 0.320 | 0.0102 | 0.0002 |
| | | 0.812 | 0.116 | ⋯ | ⋯ | 0.0099 | 0.0002 |
| | | 0.872 | 0.076 | ⋯ | ⋯ | 0.0097 | 0.0001 |
| | | 0.922 | 0.044 | ⋯ | ⋯ | 0.0099 | 0.0002 |
| | | ⋯ | ⋯ | 0.492 | 0.386 | 0.0076 | 0.0002 |
| | | ⋯ | ⋯ | 0.400 | 0.455 | 0.0059 | 0.0001 |
| | | ⋯ | ⋯ | 0.241 | 0.588 | 0.0039 | 0.0001 |
| | | ⋯ | ⋯ | 0.116 | 0.678 | 0.0017 | 0.0001 |
| 16.0 | 289.2 | 0.714 | 0.195 | 0.595 | 0.300 | 0.0102 | 0.0002 |
| | | 0.763 | 0.158 | ⋯ | ⋯ | 0.0099 | 0.0002 |
| | | 0.798 | 0.134 | ⋯ | ⋯ | 0.0099 | 0.0001 |
| | | 0.843 | 0.099 | ⋯ | ⋯ | 0.0097 | 0.0001 |
| | | 0.879 | 0.073 | ⋯ | ⋯ | 0.0099 | 0.0001 |
| | | 0.914 | 0.048 | ⋯ | ⋯ | 0.0102 | 0.0001 |
| | | 0.967 | 0.021 | ⋯ | ⋯ | 0.0104 | 0.0001 |
| | | ⋯ | ⋯ | 0.541 | 0.346 | 0.0086 | 0.0002 |
| | | ⋯ | ⋯ | 0.482 | 0.395 | 0.0071 | 0.0002 |
| | | ⋯ | ⋯ | 0.402 | 0.458 | 0.0056 | 0.0001 |
| | | ⋯ | ⋯ | 0.327 | 0.516 | 0.0041 | 0.0001 |
| | | ⋯ | ⋯ | 0.238 | 0.586 | 0.0029 | 0.0001 |
| | | ⋯ | ⋯ | 0.113 | 0.668 | 0.0017 | 0.0001 |

*The compilers extracted these data from published graphs.

## Auxiliary Information

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures of the liquid phase were determined by the synthetic method.[1] The analytical method described in Nikurashina and Mertslin[2] was used for determining equilibrium liquid phase compositions. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; purity not specified; distilled; $n(20°C,D)=1.3905$, $d(20\,°C, 4\,°C)=1.0525$.
(2) Source not specified, purity not specified; distilled; $n(20\,°C,D)=1.4370$, $d(20\,°C, 4\,°C)=0.8300$.
(3) $n(20\,°C,D)=1.333$.

**Estimated Error:**

Not specified.

**References:**

[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).
[2]N. I. Nikurashina and R. V. Mertslin, *Method of Secants* (in Russian) (Saratov University Press, 1969).

## 4.6. 1-Dodecanol

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**

I. K. Zhuravleva, E. F. Zhuravlev, and L. N. Salamatin, Zh. Obshch. Khim. **46**, 1210–4 (1976).

**Variables:**

$T$/K = 286–472

**Prepared By:**

V. P. Sazonov and N. V. Sazonov

### Experimental Data

The solubility temperatures were determined in ternary mixtures with a constant mass content of (3), respectively 20, 30, 40, 45, and 50 mass % and in ternary mixtures with constant mass relationship of (1) and (2) as 10:90, 20:80, 30:70, 40:60, 50:50, 60:40, 70:30, 80:20, and 90:10, respectively. These data are also presented in graphical form (see Tables 1–5).

Table 1. Solubility temperatures of the three liquid phases*

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass content of water=20.0 | | | |
| 16.5 | 289.7 | 72.0 | 8.0 | 0.454 | 0.020 |
| 20.0 | 293.2 | 32.0 | 48.0 | 0.238 | 0.144 |
| 21.7 | 294.9 | 68.0 | 12.0 | 0.436 | 0.031 |
| 23.4 | 296.6 | 36.0 | 24.0 | 0.263 | 0.129 |
| 24.6 | 297.8 | 64.0 | 16.0 | 0.416 | 0.042 |
| 25.5 | 298.7 | 40.0 | 40.0 | 0.287 | 0.116 |
| 26.2 | 299.4 | 60.0 | 20.0 | 0.396 | 0.053 |
| 26.3 | 299.5 | 52.0 | 28.0 | 0.355 | 0.077 |
| 26.3 | 299.5 | 48.0 | 32.0 | 0.333 | 0.089 |
| 26.4 | 299.6 | 44.0 | 36.0 | 0.310 | 0.102 |
| | | constant mass content of water=30.0 | | | |
| 18.0 | 291.2 | 31.5 | 38.5 | 0.183 | 0.090 |
| 18.4 | 291.6 | 67.0 | 7.0 | 0.376 | 0.016 |
| 22.2 | 295.4 | 35.0 | 35.0 | 0.201 | 0.081 |
| 22.9 | 296.1 | 59.5 | 10.5 | 0.315 | 0.022 |
| 24.7 | 297.9 | 38.5 | 31.5 | 0.219 | 0.072 |
| 25.3 | 298.5 | 42.0 | 28.0 | 0.236 | 0.063 |
| 25.4 | 298.6 | 56.0 | 14.0 | 0.300 | 0.030 |
| 26.2 | 299.4 | 52.5 | 17.5 | 0.285 | 0.038 |
| 26.3 | 299.5 | 49.0 | 21.0 | 0.269 | 0.046 |
| 26.4 | 299.6 | 45.5 | 24.5 | 0.252 | 0.055 |
| | | constant mass content of water=40.0 | | | |
| 13.8 | 286.0 | 57.0 | 3.0 | 0.254 | 0.005 |
| 15.8 | 289.0 | 30.0 | 30.0 | 0.144 | 0.058 |
| 19.9 | 293.1 | 54.0 | 6.0 | 0.242 | 0.010 |
| 20.4 | 293.6 | 33.0 | 27.0 | 0.157 | 0.052 |
| 23.5 | 296.7 | 36.0 | 24.0 | 0.170 | 0.046 |
| 23.8 | 297.0 | 51.0 | 9.0 | 0.231 | 0.016 |
| 25.4 | 298.6 | 39.0 | 21.0 | 0.182 | 0.040 |
| 26.3 | 299.5 | 48.0 | 12.0 | 0.219 | 0.022 |
| 26.3 | 299.5 | 42.0 | 18.0 | 0.195 | 0.034 |
| 26.4 | 299.6 | 45.0 | 15.0 | 0.207 | 0.028 |

Table 2. Solubility temperatures of the two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| | | constant mass content of water=45.0 | | | |
| 170.5 | 443.7 | 55.0 | 0.0 | 0.227 | 0.0 |
| 177.0 | 450.2 | 54.45 | 0.55 | 0.225 | 0.001 |
| 185.0 | 458.2 | 53.90 | 1.10 | 0.223 | 0.002 |
| 192.0 | 465.2 | 53.35 | 1.65 | 0.221 | 0.003 |
| 199.0 | 472.2 | 52.80 | 2.20 | 0.219 | 0.004 |
| | | constant mass content of water=50.0 | | | |
| 170.5 | 443.7 | 50.0 | 0.0 | 0.194 | 0.0 |
| 174.0 | 447.2 | 49.50 | 0.50 | 0.192 | 0.001 |
| 179.0 | 452.2 | 49.00 | 1.00 | 0.190 | 0.002 |
| 183.0 | 456.2 | 48.50 | 1.50 | 0.188 | 0.002 |
| 188.0 | 461.2 | 48.00 | 2.0 | 0.187 | 0.003 |

Table 3. Solubility temperatures of the solid phase*

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 13.9 | 287.1 | 57.0 | 3.0 | 0.254 | 0.005 |
| 15.8 | 289.0 | 54.0 | 6.0 | 0.242 | 0.010 |
| 16.2 | 289.4 | 51.0 | 9.0 | 0.231 | 0.016 |
| 16.3 | 289.5 | 48.0 | 12.0 | 0.219 | 0.022 |
| 16.5 | 289.7 | 45.0 | 15.0 | 0.207 | 0.028 |
| 17.0 | 290.2 | 36.0 | 24.0 | 0.170 | 0.046 |
| 17.3 | 290.5 | 33.0 | 27.0 | 0.157 | 0.052 |
| 18.2 | 291.4 | 30.0 | 30.0 | 0.144 | 0.058 |
| 20.2 | 293.4 | 27.0 | 33.0 | 0.131 | 0.064 |
| 22.5 | 295.7 | 24.0 | 36.0 | 0.117 | 0.071 |

Table 4. Solubility curves of the ternary system*

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 20.0 | 293.2 | 4.0 | 0.0 | 0.100 | 0.0 |
| | | 99.0 | 0.0 | 0.960 | 0.0 |
| | | 89.0 | 9.9 | 0.912 | 0.041 |
| | | 19.7 | 78.9 | 0.344 | 0.554 |
| | | 9.9 | 88.7 | 0.192 | 0.695 |
| | | 0.0 | 99.3 | 0.0 | 0.932 |
| 26.0 | 299.2 | 4.1 | 0.0 | 0.102 | 0.0 |
| | | 98.5 | 0.0 | 0.940 | 0.0 |
| | | 88.6 | 9.8 | 0.893 | 0.040 |
| | | 78.6 | 19.7 | 0.840 | 0.085 |
| | | 68.7 | 29.5 | 0.780 | 0.135 |
| | | 38.5 | 57.7 | 0.496 | 0.300 |
| | | 29.3 | 68.4 | 0.441 | 0.415 |
| | | 19.6 | 78.5 | 0.332 | 0.535 |
| | | 9.8 | 88.5 | 0.187 | 0.678 |
| | | 0.0 | 98.5 | 0.0 | 0.864 |
| | | 68.9 | 29.5 | 0.788 | 0.136 |
| | | 38.6 | 57.8 | 0.502 | 0.303 |
| | | 29.8 | 69.5 | 0.491 | 0.461 |

Table 5. Compositions of two and three coexisting liquid phases system nitroethane+1-dodecanol+water*

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase | | Alcohol-rich phase | | Water-rich phase | |
|---|---|---|---|---|---|---|---|
| | | 100 $w_1'$ | 100 $w_2'$ | 100 $w_1''$ | 100 $w_2''$ | 100 $w_1'''$ | 100 $w_2'''$ |
| 20.0 | 293.2 | 83.5 | 14.5 | 24.1 | 73.8 | 4.6 | 0.2 |
| | | 85.1 | 13.1 | ⋯ | ⋯ | 4.5 | 0.2 |
| | | 87.1 | 11.3 | ⋯ | ⋯ | 4.4 | 0.1 |
| | | 89.8 | 8.8 | ⋯ | ⋯ | 4.3 | 0.1 |
| | | 92.6 | 6.2 | ⋯ | ⋯ | 4.3 | 0.1 |
| | | 95.6 | 3.4 | ⋯ | ⋯ | 4.4 | 0.1 |
| | | 97.8 | 1.5 | ⋯ | ⋯ | 4.5 | 0.1 |
| | | ⋯ | ⋯ | 21.7 | 76.2 | 4.0 | 0.2 |
| | | ⋯ | ⋯ | 19.6 | 78.3 | 3.5 | 0.2 |
| | | ⋯ | ⋯ | 18.0 | 79.9 | 3.0 | 0.1 |
| | | ⋯ | ⋯ | 14.7 | 83.1 | 2.5 | 0.1 |
| | | ⋯ | ⋯ | 12.7 | 85.1 | 2.0 | 0.1 |
| | | ⋯ | ⋯ | 10.9 | 86.9 | 1.4 | 0.1 |
| | | ⋯ | ⋯ | 8.7 | 89.0 | 0.8 | 0.1 |
| | | ⋯ | ⋯ | 7.0 | 90.7 | 0.2 | 0.1 |
| 26.0 | 299.2 | 65.5 | 32.3 | 41.2 | 56.0 | 4.7 | 0.2 |
| | | 69.3 | 28.6 | ⋯ | ⋯ | 4.6 | 0.2 |
| | | 72.6 | 25.4 | ⋯ | ⋯ | 4.5 | 0.2 |
| | | 76.5 | 21.7 | ⋯ | ⋯ | 4.4 | 0.1 |
| | | 80.1 | 18.3 | ⋯ | ⋯ | 4.3 | 0.1 |
| | | 83.2 | 15.4 | ⋯ | ⋯ | 4.3 | 0.1 |
| | | 86.5 | 12.3 | ⋯ | ⋯ | 4.4 | 0.1 |
| | | 90.1 | 8.8 | ⋯ | ⋯ | 4.5 | 0.1 |
| | | 94.6 | 4.4 | ⋯ | ⋯ | 4.6 | 0.1 |
| | | ⋯ | ⋯ | 36.2 | 61.0 | 4.1 | 0.2 |
| | | ⋯ | ⋯ | 32.7 | 64.7 | 3.6 | 0.2 |
| | | ⋯ | ⋯ | 28.8 | 68.8 | 3.1 | 0.2 |
| | | ⋯ | ⋯ | 24.3 | 73.5 | 2.6 | 0.1 |
| | | ⋯ | ⋯ | 20.2 | 77.8 | 2.0 | 0.1 |
| | | ⋯ | ⋯ | 16.2 | 81.9 | 1.5 | 0.1 |
| | | ⋯ | ⋯ | 11.6 | 86.6 | 1.0 | 0.1 |
| | | ⋯ | ⋯ | 7.1 | 91.2 | 0.6 | 0.1 |
| | | ⋯ | ⋯ | 3.9 | 94.5 | 0.2 | 0.1 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) | | Alcohol-rich phase (compilers) | | Water-rich phase (compilers) | |
|---|---|---|---|---|---|---|---|
| | | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ | $x_1'''$ | $x_2'''$ |
| 20.0 | 293.2 | 0.850 | 0.059 | 0.385 | 0.475 | 0.0115 | 0.0002 |
| | | 0.870 | 0.054 | ⋯ | ⋯ | 0.0112 | 0.0002 |
| | | 0.886 | 0.046 | ⋯ | ⋯ | 0.0109 | 0.0001 |
| | | 0.905 | 0.036 | ⋯ | ⋯ | 0.0107 | 0.0001 |
| | | 0.925 | 0.025 | ⋯ | ⋯ | 0.0107 | 0.0001 |
| | | 0.945 | 0.014 | ⋯ | ⋯ | 0.0109 | 0.0001 |
| | | 0.965 | 0.006 | ⋯ | ⋯ | 0.0112 | 0.0001 |
| | | ⋯ | ⋯ | 0.355 | 0.502 | 0.0099 | 0.0002 |
| | | ⋯ | ⋯ | 0.327 | 0.527 | 0.0086 | 0.0001 |
| | | ⋯ | ⋯ | 0.305 | 0.546 | 0.0074 | 0.0001 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | ⋯ | ⋯ | 0.256 | 0.584 | 0.0061 | 0.0001 |
| | | ⋯ | ⋯ | 0.226 | 0.611 | 0.0049 | 0.0001 |
| | | ⋯ | ⋯ | 0.198 | 0.636 | 0.0034 | 0.0001 |
| | | ⋯ | ⋯ | 0.161 | 0.662 | 0.0019 | 0.0001 |
| | | ⋯ | ⋯ | 0.132 | 0.688 | 0.0005 | 0.0001 |
| 26.0 | 299.2 | 0.747 | 0.148 | 0.546 | 0.299 | 0.0117 | 0.0002 |
| | | 0.774 | 0.129 | ⋯ | ⋯ | 0.0115 | 0.0002 |
| | | 0.796 | 0.112 | ⋯ | ⋯ | 0.0112 | 0.0002 |
| | | 0.825 | 0.094 | ⋯ | ⋯ | 0.0109 | 0.0001 |
| | | 0.851 | 0.078 | ⋯ | ⋯ | 0.0107 | 0.0001 |
| | | 0.874 | 0.065 | ⋯ | ⋯ | 0.0107 | 0.0001 |
| | | 0.897 | 0.051 | ⋯ | ⋯ | 0.0109 | 0.0001 |
| | | 0.917 | 0.036 | ⋯ | ⋯ | 0.0112 | 0.0001 |
| | | 0.941 | 0.018 | ⋯ | ⋯ | 0.0115 | 0.0001 |
| | | ⋯ | ⋯ | 0.500 | 0.339 | 0.0102 | 0.0002 |
| | | ⋯ | ⋯ | 0.470 | 0.375 | 0.0089 | 0.0002 |
| | | ⋯ | ⋯ | 0.433 | 0.417 | 0.0076 | 0.0001 |
| | | ⋯ | ⋯ | 0.385 | 0.469 | 0.0064 | 0.0001 |
| | | ⋯ | ⋯ | 0.337 | 0.524 | 0.0049 | 0.0001 |
| | | ⋯ | ⋯ | 0.284 | 0.578 | 0.0036 | 0.0001 |
| | | ⋯ | ⋯ | 0.215 | 0.646 | 0.0024 | 0.0001 |
| | | ⋯ | ⋯ | 0.139 | 0.722 | 0.0014 | 0.0001 |
| | | ⋯ | ⋯ | 0.080 | 0.783 | 0.0005 | 0.0001 |

*The compilers extracted these data from published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Two methods were used. The solubility temperatures are determined by the synthetic method.[1] The analytical method was used for determining of equilibrium liquid phase composition. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**
(2) Source not specified; purity not specified; boiling point=114.0 °C, $n$(20 °C,D)=1.3905, $d$(20 °C,4 °C)=1.0525.
(2) Source not specified, purity not specified; boiling point=225 °C; melting point=22.6 °C, $n$(24 °C,D)=1.4420, $d$(24 °C,4 °C)=0.8310.
(3) Twice distilled; $n$(20 °C,D)=1.333.

**Estimated Error:**
Not specified.

**References:**
[1]V. F. Alekseev, Zh. Russ. Fiz.-Khim. O-va **8**, 249 (1876).

## 5. Ternary Systems Nitroethane+Two Organic Compounds

### 5.1. 1,2-Ethanediol+1-Nonanol

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]
(3) 1-Nonanol; $C_9H_{20}O$; [143-08-8]

**Original Measurements:**
I. K. Zhuravleva and L.M. Zhukova, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **20**, 516–8 (1977).

**Variables:**
$T$/K=255–329

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**
The temperatures solubility of liquid phases were determined in ternary mixtures with a constant mass relationship of (2) and (3) as 10.0:90.0, 25.3:74.7, 40.0:60.0, 55.0:45.0, 70.0:30.0, and 85.0:15.0, respectively. These data are also presented in graphical form (see Tables 1 and 2).

Table 1. Solubility temperatures of the liquid phases[a]

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship 1,2-ethanediol:1-nonanol=10.0:90.0 | | | | | |
| −15.0* | 258.2 | 8.2 | 9.2 | 0.132 | 0.178 |
| −14.0* | 259.2 | 5.0 | 9.5 | 0.082 | 0.188 |
| −11.5* | 261.7 | 0.0 | 10.0 | 0.0 | 0.205 |
| −11.2 | 262.0 | 13.3 | 8.7 | 0.207 | 0.163 |
| −11.1 | 262.1 | 93.5 | 0.7 | 0.961 | 0.008 |
| −6.0 | 267.2 | 17.8 | 8.2 | 0.269 | 0.150 |
| −4.5 | 268.7 | 90.0 | 1.0 | 0.939 | 0.013 |
| 0.5 | 273.7 | 23.6 | 7.6 | 0.344 | 0.135 |
| 4.5 | 277.7 | 83.6 | 1.6 | 0.896 | 0.021 |
| 6.4 | 279.6 | 30.0 | 7.0 | 0.421 | 0.119 |
| 9.1 | 282.3 | 37.8 | 6.2 | 0.508 | 0.101 |
| 10.0 | 283.2 | 72.7 | 2.7 | 0.819 | 0.037 |
| 10.1 | 283.3 | 44.6 | 5.5 | 0.577 | 0.087 |
| 10.5 | 283.7 | 64.3 | 3.6 | 0.754 | 0.051 |
| 11.0 | 284.2 | 53.5 | 4.7 | 0.661 | 0.070 |
| constant mass relationship 1,2-ethanediol:1-nonanol=25.3:74.7 | | | | | |
| −16.0 | 257.2 | 13.8 | 21.6 | 0.188 | 0.355 |
| −14.4 | 258.8 | 15.4 | 21.2 | 0.208 | 0.346 |
| −8.0 | 265.2 | 22.5 | 19.4 | 0.295 | 0.308 |
| −1.5 | 271.7 | 27.2 | 18.2 | 0.350 | 0.284 |
| 1.2 | 274.4 | 32.3 | 16.9 | 0.408 | 0.258 |
| 3.3 | 276.5 | 36.8 | 15.8 | 0.457 | 0.237 |
| 5.0 | 278.2 | 53.5 | 11.6 | 0.624 | 0.164 |
| 5.2 | 278.4 | 63.3 | 9.2 | 0.714 | 0.125 |
| 11.6 | 284.8 | 75.5 | 6.1 | 0.817 | 0.080 |
| 17.4 | 290.6 | 98.6 | 0.4 | 0.990 | 0.004 |
| 20.3 | 293.5 | 80.0 | 5.0 | 0.852 | 0.064 |
| 22.6 | 295.8 | 98.4 | 0.4 | 0.989 | 0.005 |
| 26.6 | 299.8 | 84.4 | 3.9 | 0.887 | 0.050 |
| 26.8 | 300.0 | 95.8 | 1.1 | 0.971 | 0.013 |
| 29.3 | 302.5 | 92.1 | 2.0 | 0.944 | 0.025 |
| 29.4 | 302.6 | 88.4 | 2.9 | 0.917 | 0.036 |
| constant mass relationship 1,2-ethanediol:1-nonanol=40.0:60.0 | | | | | |
| −17.0* | 256.2 | 17.5 | 33.0 | 0.210 | 0.480 |

| | | | | | |
|---|---|---|---|---|---|
| −15.1* | 258.1 | 12.2 | 35.1 | 0.149 | 0.517 |
| −14.2* | 259.0 | 10.5 | 35.8 | 0.129 | 0.530 |
| −13.8* | 259.4 | 22.6 | 31.0 | 0.268 | 0.445 |
| −13.0* | 260.2 | 8.2 | 36.7 | 0.101 | 0.546 |
| −12.5* | 260.7 | 5.0 | 38.0 | 0.062 | 0.570 |
| −10.5 | 262.7 | 2.2 | 39.1 | 0.028 | 0.591 |
| −8.6 | 264.6 | 26.0 | 29.6 | 0.306 | 0.422 |
| −5.8 | 267.4 | 1.6 | 39.4 | 0.020 | 0.596 |
| −3.3 | 269.9 | 30.6 | 27.8 | 0.357 | 0.391 |
| 0.0 | 273.2 | 0.0 | 40.0 | 0.0 | 0.608 |
| 1.1 | 274.3 | 39.0 | 24.4 | 0.445 | 0.337 |
| 1.9 | 275.1 | 44.0 | 22.4 | 0.497 | 0.306 |
| 2.7 | 275.9 | 50.5 | 19.8 | 0.562 | 0.266 |
| 2.9 | 276.1 | 59.5 | 16.2 | 0.649 | 0.214 |
| 2.9 | 276.1 | 66.5 | 13.4 | 0.714 | 0.174 |
| 4.7 | 277.9 | 72.1 | 11.2 | 0.765 | 0.143 |
| 6.8 | 280.0 | 77.0 | 9.2 | 0.808 | 0.117 |
| 11.4 | 284.6 | 80.0 | 8.0 | 0.834 | 0.101 |
| 14.0 | 287.2 | 95.0 | 2.0 | 0.960 | 0.024 |
| 15.8 | 289.0 | 82.3 | 7.1 | 0.854 | 0.089 |
| 21.3 | 294.5 | 92.0 | 3.2 | 0.935 | 0.039 |
| 22.1 | 295.3 | 88.4 | 4.6 | 0.905 | 0.058 |
| constant mass relationship 1,2-ethanediol:1-nonanol=55.0:45.0 | | | | | |
| −16.0* | 257.2 | 14.0 | 47.3 | 0.153 | 0.626 |
| −15.2* | 258.0 | 12.0 | 48.4 | 0.132 | 0.642 |
| −14.0* | 259.2 | 10.3 | 49.3 | 0.113 | 0.656 |
| −13.0* | 260.2 | 8.2 | 50.5 | 0.090 | 0.673 |
| −11.0 | 262.2 | 4.6 | 52.5 | 0.051 | 0.702 |
| −7.6 | 265.6 | 4.0 | 52.8 | 0.044 | 0.707 |
| −4.6 | 268.6 | 3.7 | 53.0 | 0.041 | 0.709 |
| −2.6 | 270.6 | 28.9 | 39.1 | 0.311 | 0.509 |
| 5.3 | 278.5 | 2.0 | 53.9 | 0.022 | 0.723 |
| 7.6 | 280.8 | 53.2 | 25.7 | 0.558 | 0.327 |
| 8.9 | 282.1 | 57.6 | 23.3 | 0.602 | 0.295 |
| 15.0 | 288.2 | 0.0 | 55.0 | 0.0 | 0.740 |
| 16.1 | 289.3 | 64.8 | 19.4 | 0.672 | 0.243 |
| 18.6 | 291.8 | 96.2 | 2.1 | 0.966 | 0.025 |
| 22.9 | 296.1 | 68.5 | 17.3 | 0.707 | 0.216 |
| 31.8 | 305.0 | 72.4 | 15.2 | 0.745 | 0.189 |
| 31.9 | 305.1 | 93.6 | 3.5 | 0.942 | 0.043 |
| 37.4 | 310.6 | 90.0 | 5.5 | 0.909 | 0.067 |
| 38.7 | 311.9 | 77.6 | 12.3 | 0.794 | 0.152 |
| 42.2 | 315.4 | 83.8 | 8.9 | 0.852 | 0.110 |
| constant mass relationship 1,2-ethanediol:1-nonanol=70.0:30.0 | | | | | |
| −17.0* | 256.2 | 17.5 | 57.8 | 0.175 | 0.697 |
| −14.4* | 258.8 | 15.4 | 59.2 | 0.154 | 0.715 |
| −10.8* | 262.4 | 7.8 | 64.5 | 0.078 | 0.779 |
| −8.0 | 265.2 | 22.6 | 54.2 | 0.226 | 0.654 |
| −7.5 | 265.7 | 5.6 | 66.1 | 0.056 | 0.797 |
| −1.8 | 271.4 | 27.2 | 51.0 | 0.272 | 0.615 |
| −0.9 | 272.3 | 4.2 | 67.1 | 0.042 | 0.809 |
| 3.0 | 276.2 | 31.0 | 48.3 | 0.309 | 0.583 |
| 8.0 | 281.2 | 2.2 | 68.5 | 0.022 | 0.826 |
| 9.0 | 282.2 | 38.0 | 43.4 | 0.379 | 0.524 |
| 12.1 | 285.3 | 39.5 | 42.4 | 0.394 | 0.511 |
| 15.9 | 289.1 | 45.0 | 38.5 | 0.449 | 0.465 |
| 18.7 | 291.9 | 0.0 | 70.0 | 0.0.0 | 0.844 |
| 20.8 | 294.0 | 50.5 | 34.7 | 0.504 | 0.419 |
| 27.9 | 301.1 | 96.2 | 2.7 | 0.962 | 0.032 |
| 28.0 | 301.2 | 55.0 | 31.5 | 0.549 | 0.381 |
| 38.0 | 311.2 | 61.3 | 27.1 | 0.612 | 0.327 |
| 38.0 | 311.2 | 93.8 | 4.3 | 0.938 | 0.053 |
| 42.5 | 315.7 | 65.5 | 24.2 | 0.654 | 0.292 |
| 42.7 | 315.9 | 92.2 | 5.5 | 0.922 | 0.066 |
| 46.6 | 319.8 | 70.0 | 21.0 | 0.699 | 0.254 |
| 47.0 | 320.2 | 88.4 | 8.1 | 0.884 | 0.098 |
| 50.0 | 323.2 | 76.4 | 16.5 | 0.763 | 0.200 |
| 50.4 | 323.6 | 81.1 | 13.2 | 0.811 | 0.160 |
| constant mass relationship 1,2-ethanediol:1-nonanol=85.0:15.0 | | | | | |
| −18.5* | 254.7 | 16.5 | 71.0 | 0.152 | 0.789 |
| −17.7* | 255.5 | 14.0 | 73.1 | 0.128 | 0.810 |
| −16.5* | 256.7 | 11.0 | 75.7 | 0.101 | 0.836 |
| −11.0* | 262.2 | 7.8 | 78.4 | 0.071 | 0.863 |
| −3.4 | 269.8 | 6.2 | 79.7 | 0.056 | 0.877 |
| −2.6 | 270.6 | 23.1 | 65.4 | 0.214 | 0.731 |
| −0.8 | 272.4 | 5.5 | 80.3 | 0.050 | 0.883 |
| 5.0 | 278.2 | 4.3 | 81.3 | 0.039 | 0.893 |
| 8.0 | 281.2 | 27.1 | 62.0 | 0.252 | 0.696 |
| 15.0 | 288.2 | 3.0 | 82.5 | 0.027 | 0.904 |
| 16.3 | 289.5 | 97.6 | 2.0 | 0.974 | 0.025 |
| 20.0 | 293.2 | 35.0 | 55.3 | 0.327 | 0.625 |
| 20.6 | 293.8 | 0.0 | 85.0 | 0.0 | 0.929 |
| 27.0 | 300.2 | 40.0 | 51.0 | 0.376 | 0.580 |
| 27.6 | 300.8 | 97.4 | 2.2 | 0.971 | 0.027 |
| 35.6 | 308.8 | 46.4 | 45.6 | 0.439 | 0.521 |
| 40.5 | 313.7 | 95.0 | 4.3 | 0.945 | 0.051 |
| 40.6 | 313.8 | 51.5 | 41.2 | 0.490 | 0.474 |
| 47.2 | 320.4 | 92.2 | 6.6 | 0.914 | 0.080 |
| 47.3 | 320.5 | 60.5 | 33.6 | 0.581 | 0.390 |
| 51.0 | 324.2 | 67.5 | 27.6 | 0.653 | 0.323 |
| 53.5 | 326.7 | 86.4 | 11.6 | 0.852 | 0.138 |
| 54.2 | 327.4 | 74.4 | 21.8 | 0.724 | 0.256 |
| 55.6 | 328.8 | 79.8 | 17.2 | 0.781 | 0.203 |

*Solubility temperatures of the solid phase.

Table 2. Composition of equilibrium liquid phases of the two partially miscible regions[a]

| | | Nitroethane-rich phase (compilers) | | Glycol-rich phase (compilers) | | Nitroethane-rich phase | | Glycol-rich phase | |
|---|---|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ | 100 $w_1'$ | 100 $w_2'$ | 100 $w_1''$ | 100 $w_2''$ |
| 5.0 | 278.2 | 0.977 | 0.007 | 0.175 | 0.798 | 96.5 | 0.6 | 19.8 | 74.4 |
| | | 0.944 | 0.025 | 0.262 | 0.616 | 92.1 | 2.0 | 26.1 | 50.6 |
| | | 0.923 | 0.039 | 0.320 | 0.589 | 89.8 | 3.1 | 32.6 | 49.6 |
| | | 0.894 | 0.058 | 0.427 | 0.454 | 86.4 | 4.6 | 41.4 | 36.4 |
| | | 0.838 | 0.087 | 0.508 | 0.353 | 79.5 | 6.8 | 47.6 | 27.3 |
| | | 0.894 | 0.014 | 0.354 | 0.070 | 82.7 | 1.1 | 23.3 | 3.8 |
| | | 0.880 | 0.029 | 0.440 | 0.143 | 81.5 | 2.2 | 32.4 | 8.7 |
| | | 0.834 | 0.061 | 0.570 | 0.146 | 76.7 | 4.6 | 46.1 | 9.8 |

[a]The compilers extracted these data from published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures of the liquid phase were determined by the synthetic method. The analytical method described in Nikurashina and Mertslin[1] was used for determining equilibrium liquid phase compositions. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; purity not specified; boiling point=114 °C, $n$(20 °C,D)=1.3910, $d$(20 °C,4 °C)=1.0520.
(2) Source not specified; purity not specified; $n$(20 °C,D) =1.4315, $d$(20 °C,4 °C)=1.1550.
(3) Source not specified; purity not specified; boiling point=213 °C, melting point=5.3 °C,$n$(20 °C,D)=1.4310, $d$(20 °C,4 °C)=0.8280.

**Estimated Error:**

Not specified.

**References:**

[1]N. I. Nikurashina and R. V. Mertslin, *Method of Secants* (in Russian) (Saratov University Press, 1969).

## 5.2. 1,2-Ethanol+1-Decanol

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]
(3) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

**Original Measurements:**

A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

**Variables:**

$T$/K=273–283

**Prepared By:**

V. P. Sazonov and N. I. Lisov

**Experimental Data**

Table 1. Solubility of nitroethane (1), 1,2-ethanediol (2) and 1-decanol (3)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 0.0 | 273.2 | 84 | 4 | 0.89 | 0.05 |
| | | 28.5 | 34.5 | 0.325 | 0.475 |
| | | 11[a] | 60 | 0.11 | 0.75 |
| | | 10 | 13 | 0.16 | 0.25 |
| | | 9 | 80 | 0.08 | 0.87 |
| | | 8.5 | 46.5 | 0.10 | 0.653 |
| 6.0 | 279.2 | 54[b] | 24 | 0.58 | 0.31 |
| | | 50 | 24 | 0.55 | 0.32 |
| | | 45 | 32.5 | 0.47 | 0.414 |
| | | 34 | 16 | 0.44 | 0.25 |
| | | 19 | 71 | 0.17 | 0.78 |
| | | 10[a] | 61 | 0.10 | 0.76 |
| | | 8 | 80 | 0.07 | 0.88 |
| | | 7.5 | 47.5 | 0.087 | 0.666 |
| 10.0 | 283.2 | 82 | 8 | 0.85 | 0.10 |
| | | 54[a] | 26 | 0.57 | 0.33 |
| | | 53[a] | 8 | 0.65 | 0.12 |
| | | 35 | 8 | 0.49 | 0.14 |
| | | 25 | 60 | 0.24 | 0.69 |
| | | 9[a] | 62 | 0.09 | 0.77 |
| | | 8 | 80 | 0.07 | 0.88 |
| | | 7.5 | 47.5 | 0.087 | 0.666 |

[a]Plait point of binodal curve.
[b]Col. A col is a point in a ternary system where two separate binodal curves meet at their respective plait points.

Table 2. Composition of equilibrium of two and three liquid phases

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase 100 $w_1'$ | Nitroethane-rich phase 100 $w_2'$ | Glycol-rich phase 100 $w_1''$ | Glycol-rich phase 100 $w_2''$ | Alcohol-rich phase 100 $w_1'''$ | Alcohol-rich phase 100 $w_2'''$ |
|---|---|---|---|---|---|---|---|
| 0.0 | 273.2 | 95 | 4 | 23 | 55 | ··· | ··· |
| | | 86 | 1 | 19 | 4 | solid | alcohol |
| | | 2 | 28 | 1.5 | 93.5 | solid | alcohol |
| 6.0 | 279.2 | 73 | 13 | 32 | 48 | ··· | ··· |
| 10.0 | 283.2 | 69 | 15 | 36 | 43 | ··· | ··· |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) $x_1'$ | Nitroethane-rich phase (compilers) $x_2'$ | Glycol-rich phase (compilers) $x_1''$ | Glycol-rich phase (compilers) $x_2''$ | Alcohol-rich phase (compilers) $x_1'''$ | Alcohol-rich phase (compilers) $x_2'''$ |
|---|---|---|---|---|---|---|---|
| 0.0 | 273.2 | 0.95 | 0.05 | 0.23 | 0.67 | ··· | ··· |
| | | 0.92 | 0.01 | 0.32 | 0.08 | solid | alcohol |
| | | 0.03 | 0.49 | 0.01 | 0.97 | solid | alcohol |
| 6.0 | 279.2 | 0.77 | 0.07 | 0.32 | 0.58 | ··· | ··· |
| 10.0 | 283.2 | 0.73 | 0.19 | 0.37 | 0.53 | ··· | ··· |

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The synthetic method was used. Observations were made after vigorous shaking in glass-stoppered tubes (15 mL capacity) immersed in water baths in large Dewar flasks. Temperature was adjusted by adding small amounts of cooler or warmer water. Filling started with 5 mL of one reagent followed by small additions of the other two, usually alternately, to maintain a trace of lower or upper layer, until the composition of a plait point was reached or the tube was full (see Tables 1 and 2).

**Source and Purity of Materials:**

(1) Eastman Kodak Co.; distilled with 30 cm column with reflux; boiling point=114–115 °C; melting point=−78 °C; $n$(20 °C,D)=1.3920, $\rho$(20 °C)=1046.9 g·L$^{-1}$.
(2) Purified by crystallization; melting point=−13.3 °C; $n$(20 °C,D)=1.4315, $\rho$(25 °C)=1110.1 g·L$^{-1}$.
(3) Purified by crystallization; melting point=6.8 °C; $n$(20 °C,D)=1.4372, $\rho$(20 °C)=831.8 g·L$^{-1}$.

**Estimated Error:**

Not specified.

## 5.3. 1,2-Ethanediol+1-Dodecanol

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]
(3) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Evaluator:**

V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

A survey of solubilities (soly) and liquid–liquid equilibrium data (equil.) for the system nitroethane +1,2-ethanediol+1-dodecanol is given in Table 1.

Table 1. Summary of experimental data for the system nitroethane +1,2-ethanediol+1-dodecanol

| Author(s) | $T$/K | Type of data[a] |
|---|---|---|
| Francis[1] | 285–297 | soly (33) |
| | 287 and 289 | equil. two and three liq phases (6) |
| Zhuravlev and Erofeeva[2] | 282–396 | soly (103) |
| | 288 | equil. two (6) and three (1) liq. phases |
| | 293 | equil. two liq. phases (10) |

[a]Number of experimental points in parentheses.

Solubility data

The system nitroethane +1,2-ethanediol+1-dodecanol includes a three-phase region. All three binary pairs of components, nitroethane +1,2-ethanediol, nitroethane +1-dodecanol and 1,2-ethanediol +1-dodecanol are partially miscible. The data for the binary systems (1)+(2) and (1)+(3) were compiled and critically evaluated in this volume. Recommended data for the system 1,2-ethanediol +1-dodecanol are not yet available. The reported values of UCST (upper critical solution temperature) of the binary systems are reported in Francis[1] and Zhuravlev and Erofeeva[2] and presented in Table 2.

Table 2. UCST (T/K) binary systems

| Binary system | Ref. 1 | Ref. 2 | Recommended values |
|---|---|---|---|
| nitroethane+1,2-ethanediol | 341.2 | 342.2 | 341.6 |
| nitroethane+1-dodecanol | 299.7 | 301.6 | 301.2 |
| 1,2-ethanediol+1-dodecanol | 408 | 408 | not specified |

Solubility data obtained by the synthetic method for the ternary system are reported in Francis[1] and Zhuravlev and Erofeeva.[2] Maximal temperature of the three-phase liquid equilibrium is reported to occur at 289.7 K (Francis[1]) and 291.8 K.[2] Thus, the tentative value is: $T_c$=291±1 K. Experimental errors were not reported in the papers. Depending on temperature the system nitroethane+1,2-ethanediol+1-dodecanol forms a miscibility gaps of Type I–IV.[3] In the temperature range 292–301.2 K,[1] where the three binary systems are partially miscible, the solubility curves correspond to Type III.[3] Below 292 K the solubility curves correspond to Type IV. A three-phase region occurs below 291 K.[1] In the temperature range 301.2–341.6 K, where the two binary systems nitroethane+1,2-ethanediol and 1-dodecanol+1,2-ethanediol are partially miscible, the solubility curves correspond to Type II.[3] Above 341.6 K this ternary system has only one partially miscible region.

Liquid–liquid equilibrium data

Compositions of the coexisting two and three liquid phases for the ternary system nitroethane+1,2-ethanediol+1-dodecanol were reported in two references. Composition of each phase at 288 and 293 K,[2] was calculated from the index of refraction-composition curve of saturated mixtures prepared at the time of saturation curve measurements and are also presented in a graphical form. Compositions of three liquid phases in equilibrium reported in Francis[1] were measured at 287 and 289 K and detailed information about experimental procedures is not reported. Experimental errors were not reported in the papers. All experimental data are considered tentative.

**References:**

[1]A. W. Francis, J. Phys. Chem. **60**, 20 (1956).
[2]E. F. Zhuravlev and L. F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10 (1968).
[3]R. E. Treybal, *Liquid Extraction* (McGraw–Hill, New York, 1963).

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$ ; [107-21-1]
(3) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**
A. W. Francis, J. Phys. Chem. **60**, 20–7 (1956).

**Variables:**
$T$/K = 285–297

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

Table 1. Solubility of nitroethane (1), 1,2-ethanediol (2) and 1-dodecanol (3)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 12.0[a] | 285.2 | 30 | 40 | 0.33 | 0.54 |
| 14.0 | 287.2 | 83 | 6 | 0.88 | 0.08 |
| metastable | | 29 | 13.5 | 0.42 | 0.238 |
| metastable | | 26 | 26 | 0.34 | 0.41 |
| metastable | | 23 | 47 | 0.25 | 0.62 |
| 16.0 | 289.2 | 82 | 8 | 0.86 | 0.10 |
| | | 54[b] | 22 | 0.60 | 0.29 |
| | | 54[b] | 14 | 0.64 | 0.20 |
| | | 40 | 15 | 0.52 | 0.24 |
| | | 30 | 42 | 0.33 | 0.55 |
| | | 22 | 51 | 0.23 | 0.65 |
| | | 19 | 45 | 0.22 | 0.62 |
| 16.5[c] | 289.7 | 54 | 23.5 | 0.59 | 0.31 |
| 20 | 293.2 | 75 | 12 | 0.79 | 0.15 |
| | | 54 | 7 | 0.69 | 0.11 |
| | | 46 | 31 | 0.50 | 0.40 |
| | | 35 | 45 | 0.36 | 0.56 |
| | | 27 | 53 | 0.27 | 0.65 |
| | | 22 | 68 | 0.20 | 0.76 |
| | | 20 | 40 | 0.24 | 0.57 |
| | | 15 | 80 | 0.13 | 0.85 |
| | | 10 | 25 | 0.15 | 0.46 |
| 21.0[d] | 294.2 | 24 | 61 | 0.23 | 0.71 |
| 24.0 | 297.2 | 75 | 12 | 0.79 | 0.15 |
| | | 54[b] | 3 | 0.72 | 0.05 |
| | | 50 | 29.5 | 0.53 | 0.380 |
| | | 40 | 41 | 0.41 | 0.51 |
| | | 32[b] | 55 | 0.31 | 0.64 |
| | | 19.5 | 55.5 | 0.202 | 0.694 |
| | | 19[b] | 64 | 0.18 | 0.75 |
| | | 16 | 36 | 0.20 | 0.55 |
| | | 13 | 80 | 0.12 | 0.86 |
| | | 12 | 28 | 0.17 | 0.48 |

[a]Quadruple point temperature. The equilibrium of three liquid phases crystals of alcohol.
[b]Plait point of binodal curve.
[c]Subcol temperature. A subcol is a point in a ternary system where a third binodal curve meets by its plait point with an isotherm of a ridge.
[d]Col temperature. A col is a point in a ternary system where two separate binodal curves meet at their respective plait points.

Table 2. Composition of equilibrium of two and three liquid phases

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase 100 $w_1'$ | Nitroethane-rich phase 100 $w_2'$ | Glycol-rich phase 100 $w_1''$ | Glycol-rich phase 100 $w_2''$ | Alcohol-rich phase 100 $w_1'''$ | Alcohol-rich phase 100 $w_2'''$ |
|---|---|---|---|---|---|---|---|
| 14.0 | 287.2 | 73 | 8 | 38 | 17 | solid | alcohol |
| | | 71 | 12 | 21 | 72 | 32 | 40 |
| | | 19.5 | 37.5 | 18 | 75 | solid | alcohol |
| 16.0 | 289.2 | 82 | 4 | 24 | 8 | solid | alcohol |
| | | 68 | 14 | 19 | 74 | 41 | 32 |
| | | 11 | 29 | 7 | 90 | solid | alcohol |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) $x_1'$ | Nitroethane-rich phase (compilers) $x_2'$ | Glycol-rich phase (compilers) $x_1''$ | Glycol-rich phase (compilers) $x_2''$ | Alcohol-rich phase (compilers) $x_1'''$ | Alcohol-rich phase (compilers) $x_2'''$ |
|---|---|---|---|---|---|---|---|
| 14.0 | 287.2 | 0.81 | 0.12 | 0.50 | 0.27 | solid | alcohol |
| | | 0.77 | 0.16 | 0.19 | 0.79 | 0.35 | 0.53 |
| | | 0.237 | 0.552 | 0.16 | 0.81 | solid | alcohol |
| 16.0 | 289.2 | 0.89 | 0.05 | 0.39 | 0.16 | solid | alcohol |
| | | 0.74 | 0.18 | 0.17 | 0.80 | 0.45 | 0.43 |
| | | 0.16 | 0.50 | 0.06 | 0.93 | solid | alcohol |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. Observations were made after vigorous shaking in glass-stoppered tubes (15 mL capacity) immersed in water baths in large Dewar flasks. Temperature was adjusted by adding small amounts of cooler or warmer water. Filling started with 5 mL of one reagent followed by small additions of the other two, usually alternately, to maintain a trace of lower or upper layer, until the composition of a plait point was reached or the tube was full (see Tables 1 and 2).

**Source and Purity of Materials:**
(1) Eastman Kodak Co.; distilled with 30 cm column with reflux; boiling point = 114–115 °C, melting point = −78 °C, $n$(20 °C,D) = 1.3920, $\rho$(20 °C) = 1046.9 g·L$^{-1}$.
(2) Source not specified; purity not specified; purified by crystallization; melting point = −13.3 °C, $n$(20 °C,D) = 1.4315, $\rho$(25 °C) = 1110.1 g·L$^{-1}$.
(3) Source not specified; purity not specified; purified by crystallization; melting point = 22.7 °C, $n$(24 °C,D) = 1.4410, $\rho$(24 °C) = 832 g·L$^{-1}$.

**Estimated Error:**
Not specified.

**Components:**

(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 1,2-Ethanediol; $C_2H_6O_2$ ; [107-21-1]
(3) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**

E. F. Zhuravlev and L. F. Erofeeva, Uch. Zap., Perm. Gos. Univ. **178**, 10–7 (1968).

**Variables:**

$T$/K= 282–396

**Prepared By:**

N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubility temperatures of liquid phases were determined in ternary mixtures with a constant mass relationship of (1) and (3) as 10.0:90.0, 20.0:80.0, 30.0:70.0, 40.0:60.0, 50.0:50.0, 60.0:40.0, 70.0:30.0, 80.0:20.0, and 90.0:10.0, respectively (see Tables 1 and 2),

Table 1. Solubility temperatures of two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship nitroethane:1-dodecanol=90.0:10.0 | | | | | |
| 17.5 | 290.7 | 16.83 | 81.30 | 0.1452 | 0.8483 |
| 36.0 | 309.2 | 22.95 | 74.50 | 0.2012 | 0.7899 |
| 43.0 | 316.2 | 81.72 | 9.20 | 0.8468 | 0.1153 |
| 51.2 | 324.4 | 32.58 | 63.80 | 0.2930 | 0.6939 |
| 52.0 | 325.2 | 75.96 | 15.60 | 0.7733 | 0.1921 |
| 55.0 | 328.2 | 41.31 | 54.10 | 0.3804 | 0.6025 |
| 56.0 | 329.2 | 70.92 | 21.20 | 0.7111 | 0.2571 |
| 57.5 | 330.7 | 66.42 | 26.20 | 0.6571 | 0.3135 |
| 57.9 | 331.1 | 58.59 | 34.90 | 0.5665 | 0.4081 |
| constant mass relationship nitroethane:1-dodecanol=80.0:20.0 | | | | | |
| 13.0 | 286.2 | 4.48 | 94.40 | 0.0376 | 0.9586 |
| 18.4 | 291.6 | 70.64 | 11.70 | 0.7686 | 0.1540 |
| 19.1 | 292.3 | 76.00 | 5.00 | 0.8472 | 0.0674 |
| 19.5 | 292.7 | 11.68 | 85.40 | 0.1006 | 0.8893 |
| 19.8 | 293.0 | 20.00 | 75.00 | 0.1774 | 0.8047 |
| 20.2 | 293.4 | 77.12 | 3.60 | 0.8642 | 0.0488 |
| 24.0 | 297.2 | 6.00 | 92.50 | 0.0506 | 0.9443 |
| 24.0 | 297.2 | 21.68 | 72.90 | 0.1935 | 0.7870 |
| 29.0 | 302.2 | 68.88 | 13.90 | 0.7436 | 0.1815 |
| 29.4 | 302.6 | 24.40 | 69.50 | 0.2200 | 0.7576 |
| 32.0 | 305.2 | 9.84 | 87.70 | 0.8442 | 0.9073 |
| 33.0 | 306.2 | 67.20 | 16.00 | 0.7201 | 0.2074 |
| 33.2 | 306.4 | 27.28 | 65.90 | 0.2486 | 0.7263 |
| 39.5 | 312.7 | 63.44 | 20.70 | 0.6687 | 0.2639 |
| 40.6 | 313.8 | 39.76 | 50.30 | 0.3801 | 0.5816 |
| 41.6 | 314.8 | 51.28 | 35.90 | 0.5135 | 0.4348 |
| constant mass relationship nitroethane:1-dodecanol=70.0:30.0 | | | | | |
| 10.6 | 283.8 | 18.62 | 73.40 | 0.1683 | 0.8026 |
| 15.0 | 288.2 | 21.21 | 69.70 | 0.1943 | 0.7722 |
| 18.1 | 291.3 | 24.43 | 65.10 | 0.2275 | 0.7332 |
| 18.2 | 291.4 | 62.09 | 11.30 | 0.7180 | 0.1580 |
| 20.2 | 293.4 | 55.23 | 21.10 | 0.6177 | 0.2826 |
| 22.8 | 296.0 | 67.06 | 4.20 | 0.8010 | 0.0607 |
| 23.5 | 296.7 | 27.86 | 60.20 | 0.2641 | 0.6903 |
| 23.6 | 296.8 | 53.90 | 23.00 | 0.5922 | 0.3056 |
| 27.9 | 301.1 | 34.93 | 50.10 | 0.3440 | 0.5967 |
| 28.9 | 302.1 | 37.52 | 46.40 | 0.3748 | 0.5605 |
| 29.1 | 302.3 | 46.83 | 33.10 | 0.4932 | 0.4216 |
| 29.6 | 302.8 | 40.95 | 41.50 | 0.4170 | 0.5111 |
| 32.0 | 305.2 | 2.73 | 96.10 | 0.0229 | 0.9732 |
| 36.0 | 306.2 | 13.93 | 80.10 | 0.1230 | 0.8557 |
| 50.0 | 323.2 | 10.43 | 85.10 | 0.0906 | 0.8938 |
| constant mass relationship nitroethane:1-dodecanol=60.0:40.0 | | | | | |
| 9.0 | 282.2 | 16.92 | 71.80 | 0.1562 | 0.8018 |
| 16.0 | 289.2 | 21.60 | 64.00 | 0.2061 | 0.7385 |
| 17.2 | 290.4 | 47.70 | 20.50 | 0.5592 | 0.2906 |
| 18.1 | 291.3 | 50.40 | 16.00 | 0.6051 | 0.2323 |
| 18.2 | 291.4 | 26.64 | 55.60 | 0.2637 | 0.6655 |
| 18.5 | 291.7 | 40.20 | 33.00 | 0.4422 | 0.4390 |
| 19.2 | 292.4 | 32.82 | 45.30 | 0.3404 | 0.5682 |
| 22.1 | 295.3 | 55.02 | 8.30 | 0.6892 | 0.1257 |
| 25.0 | 298.2 | 2.40 | 96.00 | 0.0201 | 0.9744 |
| 59.0 | 332.2 | 4.32 | 92.80 | 0.0367 | 0.9534 |
| 60.0 | 333.2 | 11.94 | 80.10 | 0.1066 | 0.8648 |
| 68.0 | 341.2 | 7.92 | 86.80 | 0.0689 | 0.9127 |
| constant mass relationship nitroethane:1-dodecanol=50.0:50.0 | | | | | |
| 10.5 | 283.7 | 27.35 | 45.30 | 0.2936 | 0.5881 |
| 11.8 | 285.0 | 32.55 | 34.90 | 0.3704 | 0.4803 |
| 13.0 | 286.2 | 36.00 | 28.00 | 0.4267 | 0.4014 |
| 16.5 | 289.7 | 40.10 | 19.80 | 0.5000 | 0.2986 |
| 19.8 | 293.0 | 43.90 | 12.20 | 0.5750 | 0.1933 |
| 20.0 | 293.2 | 21.40 | 57.20 | 0.2157 | 0.6974 |
| 23.9 | 297.1 | 47.30 | 5.40 | 0.6489 | 0.0896 |
| 43.0 | 316.2 | 16.50 | 67.00 | 0.1584 | 0.7778 |
| 60.0 | 333.2 | 12.50 | 75.00 | 0.1155 | 0.8380 |
| 72.0 | 345.2 | 5.45 | 89.10 | 0.0472 | 0.9337 |
| constant mass relationship nitroethane:1-dodecanol=40.0:60.0 | | | | | |
| 11.0 | 284.2 | 28.00 | 30.00 | 0.3448 | 0.4168 |
| 12.7 | 285.9 | 30.16 | 24.60 | 0.3860 | 0.3808 |
| 14.8 | 288.0 | 32.20 | 19.50 | 0.4279 | 0.3134 |
| 16.2 | 289.4 | 33.36 | 16.60 | 0.4533 | 0.2728 |
| 20.0 | 293.4 | 36.28 | 9.30 | 0.5224 | 0.1619 |
| 20.0 | 293.4 | 21.16 | 47.10 | 0.2328 | 0.6266 |
| 23.7 | 296.9 | 37.96 | 5.10 | 0.5660 | 0.0920 |
| 30.5 | 303.7 | 19.80 | 50.50 | 0.2133 | 0.6579 |
| 46.0 | 319.2 | 16.60 | 58.50 | 0.1705 | 0.7265 |
| 66.0 | 339.2 | 11.84 | 70.40 | 0.1137 | 0.8176 |
| 84.0 | 357.2 | 8.24 | 79.40 | 0.0754 | 0.8790 |
| 86.2 | 359.4 | 7.36 | 81.60 | 0.0666 | 0.8931 |
| constant mass relationship nitroethane:1-dodecanol=30.0:70.0 | | | | | |
| 11.0 | 284.2 | 24.99 | 16.70 | 0.3639 | 0.2941 |
| 16.5 | 289.7 | 27.09 | 9.70 | 0.4214 | 0.1825 |
| 21.0 | 294.2 | 28.53 | 4.90 | 0.4656 | 0.0967 |
| 26.0 | 299.2 | 18.18 | 39.40 | 0.2192 | 0.5747 |
| 30.0 | 303.2 | 17.37 | 42.10 | 0.2053 | 0.6017 |
| 42.0 | 315.2 | 1.50 | 95.00 | 0.0127 | 0.9753 |
| 56.5 | 329.7 | 14.19 | 52.70 | 0.1555 | 0.6984 |
| 59.0 | 332.2 | 13.77 | 54.10 | 0.1494 | 0.7101 |
| 68.1 | 341.3 | 12.72 | 57.60 | 0.1348 | 0.7384 |
| 89.5 | 362.7 | 9.00 | 70.00 | 0.0881 | 0.8290 |
| 96.0 | 369.2 | 7.32 | 75.60 | 0.0693 | 0.8656 |
| 102.0 | 375.2 | 5.58 | 81.40 | 0.0511 | 0.9009 |
| 105.0 | 378.2 | 4.23 | 85.90 | 0.0377 | 0.9268 |
| constant mass relationship nitroethane:1-dodecanol=20.0:80.0 | | | | | |
| 24.0 | 297.2 | 0.80 | 96.00 | 0.0068 | 0.9823 |

| | | | | | |
|---|---|---|---|---|---|
| 33.0 | 306.2 | 13.00 | 35.00 | 0.1704 | 0.5549 |
| 60.0 | 333.2 | 11.40 | 43.00 | 0.1394 | 0.6359 |
| 78.5 | 351.7 | 9.58 | 52.10 | 0.1088 | 0.7158 |
| 101.9 | 375.1 | 6.38 | 68.10 | 0.0644 | 0.8317 |
| 111.0 | 384.2 | 2.40 | 88.00 | 0.0213 | 0.9444 |
| 112.0 | 385.2 | 3.28 | 83.60 | 0.0299 | 0.9219 |
| constant mass relationship nitroethane:1-dodecanol=10.0:90.0 | | | | | |
| 20.0 | 293.2 | 7.70 | 23.00 | 0.1214 | 0.4345 |
| 52.0 | 325.2 | 0.30 | 97.00 | 0.0025 | 0.9883 |
| 64.5 | 337.7 | 6.60 | 34.00 | 0.0921 | 0.5739 |
| 80.5 | 353.7 | 6.14 | 38.60 | 0.0818 | 0.6217 |
| 109.0 | 382.2 | 4.74 | 52.60 | 0.0554 | 0.7437 |
| 114.0 | 387.2 | 0.79 | 92.10 | 0.0069 | 0.9682 |
| 120.5 | 393.7 | 3.65 | 63.50 | 0.0390 | 0.8198 |
| 122.0 | 395.2 | 1.34 | 86.60 | 0.0121 | 0.9441 |
| 123.0 | 396.2 | 2.09 | 79.10 | 0.0198 | 0.9082 |

Table 2. Compositions of two and three coexisting liquid phases system nitroethane+1,2-ethanediol+1-dodecanol*

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase | | Glycol-rich phase | | Alcohol-rich phase | |
|---|---|---|---|---|---|---|---|
| | | $100\ w_1'$ | $100\ w_2'$ | $100\ w_1''$ | $100\ w_2''$ | $100\ w_1'''$ | $100\ w_2'''$ |
| 15.0 | 288.2 | 77.5 | 10.2 | 17.3 | 77.4 | 38.0 | 30.7 |
| | | 85.9 | 6.9 | 17.1 | 81.7 | ··· | ··· |
| | | 91.5 | 5.8 | 16.8 | 83.0 | ··· | ··· |
| | | ··· | ··· | 17.9 | 70.3 | 22.3 | 45.9 |
| | | ··· | ··· | 12.4 | 82.7 | 18.1 | 34.7 |
| | | ··· | ··· | 9.4 | 86.0 | 10.8 | 25.1 |
| | | ··· | ··· | 4.9 | 92.8 | 5.3 | 19.9 |
| 20.0 | 293.2 | 83.9 | 0.8 | ··· | ··· | 25.8 | 2.7 |
| | | 79.3 | 3.4 | ··· | ··· | 28.2 | 6.8 |
| | | 74.1 | 5.2 | ··· | ··· | 34.2 | 11.0 |
| | | 85.6 | 6.3 | 16.6 | 81.3 | ··· | ··· |
| | | 75.5 | 10.3 | 17.2 | 79.7 | ··· | ··· |
| | | 64.8 | 14.5 | 20.2 | 73.5 | ··· | ··· |
| | | ··· | ··· | 5.4 | 92.3 | 4.3 | 20.8 |
| | | ··· | ··· | 8.6 | 87.0 | 8.2 | 24.2 |
| | | ··· | ··· | 12.5 | 81.1 | 11.3 | 29.2 |
| | | ··· | ··· | 16.6 | 74.1 | 15.5 | 34.5 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) | | Glycerine-rich phase (compilers) | | Alcohol-rich phase (compilers) | |
|---|---|---|---|---|---|---|---|
| | | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ | $x_1'''$ | $x_2'''$ |
| 15.0 | 288.2 | 0.818 | 0.130 | 0.153 | 0.828 | 0.433 | 0.423 |
| | | 0.884 | 0.086 | 0.147 | 0.849 | ··· | ··· |
| | | 0.919 | 0.070 | 0.143 | 0.856 | ··· | ··· |
| | | ··· | ··· | 0.166 | 0.790 | 0.246 | 0.613 |
| | | ··· | ··· | 0.108 | 0.874 | 0.229 | 0.531 |
| | | ··· | ··· | 0.082 | 0.902 | 0.161 | 0.453 |
| | | ··· | ··· | 0.042 | 0.951 | 0.089 | 0.405 |
| 20.0 | 293.2 | 0.922 | 0.011 | ··· | ··· | 0.446 | 0.056 |
| | | 0.877 | 0.046 | ··· | ··· | 0.450 | 0.131 |
| | | 0.835 | 0.071 | ··· | ··· | 0.492 | 0.191 |
| | | 0.887 | 0.079 | 0.143 | 0.849 | ··· | ··· |
| | | 0.806 | 0.133 | 0.150 | 0.839 | ··· | ··· |
| | | 0.715 | 0.193 | 0.179 | 0.797 | ··· | ··· |
| | | ··· | ··· | 0.046 | 0.946 | 0.072 | 0.422 |
| | | ··· | ··· | 0.074 | 0.910 | 0.127 | 0.452 |
| | | ··· | ··· | 0.110 | 0.867 | 0.160 | 0.500 |
| | | ··· | ··· | 0.151 | 0.815 | 0.200 | 0.539 |

*The compilers extracted these data from published graphs.

## Auxiliary Information

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures are determined by the synthetic method. The analytical method was used for determining of equilibrium liquid phase composition. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; pure grade reagent; distilled.
(2) Source not specified; pure grade reagent; distilled.
(3) Source not specified; pure grade reagent; distilled.

**Estimated Error:**

Not specified.

## 5.4. 1,2,3-Propanetriol+1-Dodecanol

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1,2,3-Propanetriol; $C_3H_8O_3$; [56-81-5]
(3) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]

**Original Measurements:**

L. F. Erofeeva and E. F. Zhuravlev, Uch. Zap., Perm. Gos. Univ. **178**, 18–22 (1968).

**Variables:**

$T$/K=291–455

**Prepared By:**

N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

### Experimental Data

The solubility temperatures of liquid phases were determined in ternary mixtures with a constant mass content of (2), respectively, 20.0, 50.0, and 70.0 mass % and in ternary mixtures with constant mass relationship of (1) and (3) as 10.0:90.0, 20.0:80.0, 30.0:70.0, 50.0:50.0, 80.0:20.0, and 90.0:10.0, respectively (see Tables 1 and 2).

Table 1. Solubility temperatures of two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship nitroethane:1-dodecanol=10.0:90.0 | | | | | |
| 19.2 | 292.4 | 9.65 | 3.50 | 0.2032 | 0.0601 |
| 38.0 | 311.2 | 9.62 | 3.80 | 0.2021 | 0.0651 |
| 49.0 | 322.2 | 0.11 | 98.90 | 0.0014 | 0.9937 |
| 76.0 | 349.2 | 0.20 | 98.00 | 0.0025 | 0.9886 |
| 79.8 | 353.0 | 9.51 | 4.90 | 0.1982 | 0.0832 |
| 102.0 | 375.2 | 9.42 | 5.80 | 0.1950 | 0.0979 |
| 114.0 | 387.2 | 0.29 | 97.10 | 0.0036 | 0.9833 |
| 124.0 | 397.2 | 9.36 | 6.40 | 0.1929 | 0.1075 |
| 146.0 | 419.2 | 0.33 | 96.70 | 0.0041 | 0.9810 |
| 148.0 | 421.2 | 9.18 | 8.20 | 0.1868 | 0.1360 |
| constant mass relationship nitroethane:1-dodecanol=20.0:80.0 | | | | | |
| 18.0 | 291.2 | 19.74 | 1.30 | 0.3752 | 0.0201 |
| 18.0 | 291.2 | 19.52 | 2.40 | 0.3688 | 0.0370 |
| 18.4 | 291.6 | 19.84 | 0.80 | 0.3782 | 0.0124 |
| 43.0 | 316.2 | 19.40 | 3.00 | 0.3653 | 0.0460 |
| 54.0 | 327.2 | 0.38 | 98.10 | 0.0047 | 0.9877 |
| 76.0 | 349.2 | 19.12 | 4.40 | 0.3573 | 0.0670 |
| 87.0 | 360.2 | 0.48 | 97.60 | 0.0059 | 0.9845 |
| 94.0 | 367.2 | 19.00 | 5.00 | 0.3539 | 0.0759 |
| 112.0 | 385.2 | 0.60 | 97.00 | 0.0074 | 0.9806 |
| 114.0 | 387.2 | 18.82 | 5.90 | 0.3488 | 0.0891 |
| 133.0 | 406.2 | 18.48 | 7.60 | 0.3394 | 0.1138 |
| 165.0 | 438.2 | 18.24 | 8.80 | 0.3328 | 0.1309 |
| 182.0 | 455.2 | 18.00 | 10.00 | 0.3263 | 0.1478 |
| constant mass relationship nitroethane:1-dodecanol=30.0:70.0 | | | | | |
| 25.2 | 298.4 | 29.67 | 1.10 | 0.5075 | 0.0153 |
| 51.0 | 324.2 | 29.10 | 3.00 | 0.4940 | 0.0415 |
| 52.0 | 325.2 | 0.60 | 98.00 | 0.0074 | 0.9856 |
| 81.0 | 354.2 | 0.75 | 97.50 | 0.0093 | 0.9820 |
| 82.0 | 355.2 | 28.77 | 4.10 | 0.4863 | 0.0565 |
| 97.0 | 370.2 | 28.53 | 4.90 | 0.4808 | 0.0673 |
| 103.5 | 376.7 | 0.90 | 97.00 | 0.0111 | 0.9784 |
| 110.5 | 383.7 | 28.32 | 5.60 | 0.4759 | 0.0767 |
| 134.0 | 407.2 | 27.87 | 7.10 | 0.4656 | 0.0967 |
| 157.0 | 430.2 | 27.33 | 8.90 | 0.4534 | 0.1204 |
| constant mass relationship nitroethane:1-dodecanol=50.0:50.0 | | | | | |
| 28.8 | 302.0 | 49.55 | 0.90 | 0.7054 | 0.0104 |
| 40.0 | 313.2 | 48.65 | 2.70 | 0.6905 | 0.0312 |
| 76.0 | 349.2 | 1.25 | 97.50 | 0.0154 | 0.9784 |
| 82.0 | 355.2 | 47.70 | 4.60 | 0.6750 | 0.0531 |
| 105.0 | 378.2 | 2.00 | 96.00 | 0.0247 | 0.9654 |
| 106.0 | 379.2 | 47.00 | 6.00 | 0.6636 | 0.0691 |
| constant mass relationship nitroethane:1-dodecanol=80.0:20.0 | | | | | |
| 23.0 | 296.2 | 79.68 | 0.40 | 0.9051 | 0.0037 |
| 44.0 | 317.2 | 79.20 | 1.00 | 0.9001 | 0.0093 |
| 63.0 | 336.2 | 78.82 | 1.60 | 0.8950 | 0.0148 |
| 81.0 | 354.2 | 3.20 | 96.00 | 0.0391 | 0.9569 |
| 89.0 | 362.2 | 77.68 | 2.90 | 0.8841 | 0.0269 |
| 89.0 | 362.2 | 76.88 | 3.90 | 0.8756 | 0.0362 |
| 114.0 | 387.2 | 4.00 | 95.00 | 0.0489 | 0.9462 |
| constant mass relationship nitroethane:1-dodecanol=90.0:10.0 | | | | | |
| 48.0 | 321.2 | 89.28 | 0.80 | 0.9505 | 0.0069 |
| 68.0 | 341.2 | 88.38 | 1.80 | 0.9422 | 0.0156 |
| 68.0 | 341.2 | 3.42 | 96.20 | 0.0417 | 0.9564 |
| 84.0 | 357.2 | 4.05 | 95.50 | 0.0493 | 0.9484 |
| 89.0 | 362.2 | 87.21 | 3.10 | 0.9313 | 0.0270 |
| 108.0 | 381.2 | 5.40 | 94.00 | 0.0656 | 0.9314 |
| 120.0 | 393.2 | 84.42 | 6.20 | 0.9053 | 0.0542 |

Table 2. Compositions of two and three coexisting liquid phases system nitroethane+1,2,3-propanetriol+1-dodecanol*

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase 100 $w_1'$ | Nitroethane-rich phase 100 $w_2'$ | Glycerine-rich phase 100 $w_1''$ | Glycerine-rich phase 100 $w_2''$ | Alcohol-rich phase 100 $w_1'''$ | Alcohol-rich phase 100 $w_2'''$ |
|---|---|---|---|---|---|---|---|
| 20.0 | 293.2 | 84.7 | 1.1 | 2.5 | 97.2 | 22.1 | 2.5 |
| | | 88.9 | 0.9 | 2.6 | 97.2 | ⋯ | ⋯ |
| | | 93.5 | 0.7 | 2.7 | 97.2 | ⋯ | ⋯ |
| | | ⋯ | ⋯ | 2.2 | 97.5 | 12.6 | 2.4 |
| | | ⋯ | ⋯ | 1.2 | 98.6 | 7.9 | 2.3 |
| | | ⋯ | ⋯ | 0.2 | 99.6 | 3.2 | 2.2 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) $x_1'$ | Nitroethane-rich phase (compilers) $x_2'$ | Glycerine-rich phase (compilers) $x_1''$ | Glycerine-rich phase (compilers) $x_2''$ | Alcohol-rich phase (compilers) $x_1'''$ | Alcohol-rich phase (compilers) $x_2'''$ |
|---|---|---|---|---|---|---|---|
| 20.0 | 293.2 | 0.927 | 0.010 | 0.031 | 0.968 | 0.406 | 0.037 |
| | | 0.948 | 0.008 | 0.032 | 0.967 | ⋯ | ⋯ |
| | | 0.970 | 0.006 | 0.033 | 0.967 | ⋯ | ⋯ |
| | | ⋯ | ⋯ | 0.027 | 0.972 | 0.258 | 0.040 |
| | | ⋯ | ⋯ | 0.015 | 0.984 | 0.172 | 0.041 |
| | | ⋯ | ⋯ | 0.002 | 0.996 | 0.074 | 0.042 |

*The compilers extracted these data from published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures are determined by the synthetic method. The analytical method was used for determining of equilibrium liquid phase composition. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; pure grade reagent; dried over $CaCl_2$ and distilled.
(2) Source not specified; pure grade reagent.
(3) Source not specified; pure grade reagent.

**Estimated Error:**

Not specified.

## 5.5. 2,5-Furandione+Hexane

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 2,5-Furandione; $C_4H_2O_3$; [108-31-6]
(3) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**

R. B. Snyder and C. A. Eckert, J. Chem. Eng. Data **18**, 282–5 (1973).

**Variables:**

$T$/K = 306–312

**Prepared By:**

N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility temperatures of liquid phases

| $t$/°C | $T$/K (compilers) | $x_1$ | $x_2$ | 100 $w_1$ (compilers) | 100 $w_2$ (compilers) |
|---|---|---|---|---|---|
| 32.59 | 305.74 | 0.505 84 | 0.002 29 | 47.121 | 0.279 |
| 33.81 | 306.96 | 0.504 45 | 0.005 02 | 46.963 | 0.610 |
| 34.85 | 308.00 | 0.502 94 | 0.008 00 | 46.793 | 0.972 |
| 35.63 | 308.78 | 0.502 31 | 0.009 25 | 46.721 | 1.124 |
| 36.19 | 309.34 | 0.501 93 | 0.010 00 | 46.678 | 1.215 |
| 36.32 | 309.47 | 0.501 78 | 0.010 30 | 46.661 | 1.251 |
| 38.72 | 311.87 | 0.498 38 | 0.017 00 | 46.278 | 2.062 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The synthetic method was used. The solubility temperatures were determined from a set of samples made up to composition by weight and sealed into 7 mm Pyrex tubes about 9 cm long. A short length of glass rod was placed in each tube as a stirrer. An apparatus was constructed to rotate the tube end over end inside the temperature bath, so that the glass rod stirrer would fall through the liquid, causing mixing. The apparatus consisted of a submerged horizontal drive shaft with a fuse holder perpendicularly attached to one end. The sealed glass tube was placed in the fuse holder, and the shaft was rotated by a rubber pulley connected to a 4 rpm electric motor mounted on a platform above the water level.

**Source and Purity of Materials:**

(1) Distilled in 1.5 m column packed with nichrome helices; purity 99.9 mass %.
(2) Sublimed at vacuum to remove maleic acid; purity 99.5 mass %.
(3) Distilled at a 15:1 reflux ratio in column packed with glass helices; purity 99.9 mass %; boiling point = 68.0–68.1 °C.

**Estimated Error:**

Temperature: control: ±0.01 K.

## 5.6. 2,2′-Iminobisethanol+Cyclohexane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2′-Iminobisethanol; $C_4H_{11}NO_2$ ; [111-42-2]
(3) Cyclohexane; $C_6H_{12}$ ; [110-82-7]

**Original Measurements:**
L. F. Erofeeva and N. V. Yunnikova, Sb. Nauch. Tr., Kuzbas. Polytekh. Inst. **26**, 7–11 (1971).

**Variables:**
$T$/K=279–368

**Prepared By:**
N. I. Lisov, V. P. Sazonov, and N. V. Sazonov

**Experimental Data**

The solubility temperatures of liquid phases were determined in ternary mixtures with a constant mass content of (2), respectively, 30.0, 50.0, and 70.0 mass %, and in ternary mixtures with a constant mass relationship of (1) and (3), respectively, 30.0:70.0, 50.0:50.0, 70.0:30.0, 80.0:20.0, and 90.0:10.0 (see Tables 1–3).

Table 1. Solubility temperatures of the three liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass content of 2,2′-iminobisethanol=30.0 | | | | | |
| 5.5 | 278.7 | 60.0 | 30.0 | 0.664 | 0.237 |
| 8.1 | 281.3 | 10.0 | 30.0 | 0.118 | 0.252 |
| 15.0 | 288.2 | 50.0 | 30.0 | 0.560 | 0.240 |
| 20.2 | 293.4 | 20.0 | 30.0 | 0.233 | 0.249 |
| 22.5 | 295.7 | 40.0 | 30.0 | 0.454 | 0.243 |
| 23.9 | 297.1 | 30.0 | 30.0 | 0.344 | 0.246 |
| constant mass content of 2,2′-iminobisethanol=50.0 | | | | | |
| 9.5 | 282.7 | 10.0 | 50.0 | 0.123 | 0.439 |
| 16.1 | 289.3 | 35.0 | 50.0 | 0.416 | 0.425 |
| 20.1 | 293.3 | 15.0 | 50.0 | 0.183 | 0.436 |
| 22.0 | 295.2 | 30.0 | 50.0 | 0.359 | 0.427 |
| 23.9 | 297.1 | 25.0 | 50.0 | 0.301 | 0.430 |
| 23.9 | 297.1 | 20.0 | 50.0 | 0.243 | 0.433 |
| constant mass content of 2,2′-iminobisethanol=70.0 | | | | | |
| 17.5 | 290.7 | 10.0 | 70.0 | 0.129 | 0.642 |
| 19.1 | 292.3 | 20.0 | 70.0 | 0.254 | 0.633 |
| 23.9 | 297.1 | 15.0 | 70.0 | 0.191 | 0.638 |

Table 2. Solubility temperatures of the two liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship nitroethane:cyclohexane=30.0:70.0 | | | | | |
| 40.5 | 313.7 | 0.9 | 97.0 | 0.012 | 0.962 |
| 42.0 | 315.2 | 29.9 | 0.3 | 0.324 | 0.002 |
| 60.0 | 333.2 | 1.0 | 96.5 | 0.014 | 0.955 |
| 77.0 | 350.2 | 1.5 | 95.0 | 0.021 | 0.936 |
| 81.5 | 354.7 | 29.5 | 1.5 | 0.320 | 0.012 |
| 88.0 | 361.2 | 2.4 | 92.0 | 0.033 | 0.899 |
| 89.0 | 362.2 | 29.4 | 2.0 | 0.319 | 0.016 |
| constant mass relationship nitroethane:cyclohexane=50.0:50.0 | | | | | |
| 39.0 | 312.2 | 2.5 | 95.0 | 0.034 | 0.935 |
| 56.2 | 329.4 | 49.7 | 0.6 | 0.526 | 0.005 |
| 62.0 | 335.2 | 49.4 | 1.2 | 0.524 | 0.009 |
| 80.0 | 353.2 | 4.5 | 91.0 | 0.061 | 0.884 |
| 82.0 | 363.2 | 48.3 | 3.5 | 0.514 | 0.027 |
| 90.0 | 363.2 | 47.3 | 5.5 | 0.506 | 0.042 |
| 90.0 | 363.2 | 5.0 | 90.0 | 0.068 | 0.872 |
| constant mass relationship nitroethane:cyclohexane=70.0:30.0 | | | | | |
| 49.0 | 322.2 | 7.0 | 90.0 | 0.095 | 0.869 |
| 63.5 | 336.7 | 68.9 | 1.6 | 0.715 | 0.012 |
| 77.0 | 350.2 | 68.3 | 2.5 | 0.710 | 0.019 |
| 80.0 | 353.2 | 9.8 | 86.0 | 0.131 | 0.819 |
| 90.0 | 363.2 | 10.9 | 84.5 | 0.145 | 0.801 |
| 91.0 | 364.2 | 66.1 | 5.6 | 0.693 | 0.042 |
| constant mass relationship nitroethane:cyclohexane=80.0:20.0 | | | | | |
| 33.5 | 306.7 | 10.8 | 86.5 | 0.144 | 0.824 |
| 43.6 | 316.8 | 79.0 | 1.2 | 0.810 | 0.009 |
| 62.5 | 335.7 | 78.3 | 2.1 | 0.805 | 0.015 |
| 79.0 | 352.2 | 76.4 | 4.5 | 0.791 | 0.033 |
| 82.0 | 355.2 | 20.0 | 75.0 | 0.256 | 0.686 |
| 89.0 | 362.2 | 72.9 | 8.9 | 0.763 | 0.067 |
| 90.0 | 363.2 | 23.2 | 71.0 | 0.293 | 0.641 |
| constant mass relationship nitroethane:cyclohexane=90.0:10.0 | | | | | |
| 33.2 | 306.4 | 20.4 | 77.3 | 0.263 | 0.711 |
| 51.0 | 324.2 | 21.9 | 75.7 | 0.280 | 0.692 |
| 59.5 | 332.7 | 88.5 | 1.7 | 0.899 | 0.012 |
| 60.0 | 333.2 | 23.4 | 74.0 | 0.298 | 0.673 |
| 70.0 | 343.2 | 26.6 | 70.4 | 0.334 | 0.632 |
| 71.8 | 345.0 | 85.6 | 4.9 | 0.877 | 0.036 |
| 80.0 | 353.2 | 31.6 | 64.9 | 0.390 | 0.572 |
| 82.1 | 355.3 | 81.3 | 9.7 | 0.845 | 0.072 |
| 85.9 | 359.1 | 36.0 | 60.0 | 0.437 | 0.520 |
| 87.2 | 360.4 | 76.4 | 15.1 | 0.806 | 0.114 |
| 90.1 | 363.3 | 71.5 | 20.5 | 0.767 | 0.157 |
| 92.1 | 365.3 | 45.0 | 50.0 | 0.529 | 0.419 |
| 95.0 | 368.2 | 63.0 | 30.0 | 0.695 | 0.236 |
| 95.0 | 368.2 | 54.0 | 40.0 | 0.614 | 0.325 |

Table 3. Compositions of two and three coexisting liquid phases system*

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase 100 $w_1'$ | Nitroethane-rich phase 100 $w_2'$ | Iminobisethanol-rich phase 100 $w_1''$ | Iminobisethanol-rich phase 100 $w_2''$ | Hydrocarbon-rich phase 100 $w_1'''$ | Hydrocarbon-rich phase 100 $w_2'''$ |
|---|---|---|---|---|---|---|---|
| 20.0 | 293.2 | 61.4 | 0.7 | 7.2 | 90.9 | 23.7 | 0.6 |
| | | 67.5 | 0.7 | 12.4 | 86.2 | ··· | ··· |
| | | 75.7 | 0.8 | 17.5 | 81.4 | ··· | ··· |
| | | 86.1 | 1.0 | 20.6 | 78.4 | ··· | ··· |
| | | ··· | ··· | 3.3 | 94.8 | 16.5 | 0.5 |
| | | ··· | ··· | 1.6 | 96.9 | 7.2 | 0.4 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Nitroethane-rich phase (compilers) $x_1'$ | Nitroethane-rich phase (compilers) $x_2'$ | Iminobisethanol-rich phase (compilers) $x_1''$ | Iminobisethanol-rich phase (compilers) $x_2''$ | Hydrocarbon-rich phase (compilers) $x_1'''$ | Hydrocarbon-rich phase (compilers) $x_2'''$ |
|---|---|---|---|---|---|---|---|
| 20.0 | 293.2 | 0.642 | 0.005 | 0.098 | 0.879 | 0.259 | 0.005 |
| | | 0.701 | 0.005 | 0.165 | 0.818 | ··· | ··· |
| | | 0.778 | 0.006 | 0.228 | 0.759 | ··· | ··· |
| | | 0.876 | 0.007 | 0.266 | 0.723 | ··· | ··· |
| | | ··· | ··· | 0.045 | 0.931 | 0.181 | 0.004 |
| | | ··· | ··· | 0.022 | 0.959 | 0.080 | 0.003 |

*The compilers extracted these data from published graphs.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Two methods were used. The solubility temperatures are determined by the synthetic method. The analytical method was used for determining equilibrium liquid phase composition. Samples from coexisting liquid phases at equilibrium were analyzed by refractometry. No experimental details given.

**Source and Purity of Materials:**

(1) Source not specified; pure grade reagent; distilled.
(2) Source not specified; pure grade reagent.
(3) Source not specified; pure grade reagent; distilled.

**Estimated Error:**

Not specified.

## 5.7. 2-Methyl-1,3-butadiene+Hexane

**Components:**

(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 2-Methyl-1,3-butadiene; $C_5H_8$; [78-79-5]
(3) Hexane; $C_6H_{14}$; [110-54-3]

**Original Measurements:**

R. B. Snyder and C. A. Eckert, J. Chem. Eng. Data **18**, 282–5 (1973).

**Variables:**

$T$/K = 301–304

**Prepared By:**

N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility temperatures of the liquid phases

| $t$/°C | $T$/K (compilers) | $x_1$ | $x_2$ | 100 $w_1$ (compilers) | 100 $w_2$ (compilers) |
|---|---|---|---|---|---|
| 27.57 | 300.72 | 0.493 06 | 0.027 50 | 46.149 | 2.336 |
| 28.77 | 301.92 | 0.495 87 | 0.021 95 | 46.372 | 1.863 |
| 29.51 | 302.66 | 0.499 65 | 0.014 50 | 46.672 | 1.229 |
| 29.78 | 302.93 | 0.500 22 | 0.013 38 | 46.717 | 1.134 |
| 30.88 | 304.03 | 0.504 47 | 0.005 00 | 47.052 | 0.423 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The synthetic method was used. The solubility temperatures were determined from a set of samples made up to composition by weight and sealed into 7 mm Pyrex tubes about 9 cm long. A short length of glass rod was placed in each tube as a stirrer. An apparatus was constructed to rotate the tube end over end inside the temperature bath, so that the glass rod stirrer would fall through the liquid, causing mixing. The apparatus consisted of a submerged horizontal drive shaft with a fuse holder perpendicularly attached to one end. The sealed glass tube was placed in the fuse holder, and the shaft was rotated by a rubber pulley connected to a 4 rpm electric motor mounted on a platform above the water level.

**Source and Purity of Materials:**

(1) Distilled in 1.5 m column packed with nichrome helices; purity 99.9 mass %.
(2) Distilled in 0.5 m column packed with nichrome helices; purity 99.7 mass %.
(3) Distilled at a 15:1 reflux ratio in 1 m column packed with glass helices; purity 99.9 mass %; boiling point=68.0–68.1 °C.

**Estimated Error:**

Temperature: control: ±0.01 K.

## 5.8. Nitrobenzene+Hexane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Nitrobenzene; $C_6H_5NO_2$ ; [98-95-3]
(3) Hexane; $C_6H_{14}$ ; [110-54-3]

**Original Measurements:**
J. Ziolo, Z. Ziejewska, and J. Piotrowska, J. Phys. Chem. **84**, 979–80 (1980).

**Variables:**
$T$/K=290–301

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The solubility temperatures of the liquid phases of ternary system over the temperature range are presented in the original publication in graphical form. The data from this table were extracted by the compilers from published graphs.

Solubility temperatures of the liquid phases

| $t$/°C | $T$/K (compilers) | $x_1$ | $x_2$ | 100 $w_1$ (compilers) | 100 $w_2$ (compilers) |
|---|---|---|---|---|---|
| 16.6 | 289.8 | 0.227 | 0.339 | 17.7 | 43.4 |
| 16.7 | 289.9 | 0.170 | 0.397 | 12.9 | 49.4 |
| 17.0 | 290.2 | 0.299 | 0.266 | 24.2 | 35.3 |
| 17.1 | 290.3 | 0.122 | 0.446 | 9.0 | 54.2 |
| 17.6 | 290.8 | 0.338 | 0.226 | 28.0 | 30.7 |
| 17.9 | 291.1 | 0.357 | 0.206 | 29.8 | 28.2 |
| 18.2 | 291.4 | 0.041 | 0.528 | 2.9 | 61.8 |
| 19.1 | 292.3 | 0.000 | 0.570 | 0.0 | 65.4 |
| 19.1 | 292.3 | 0.405 | 0.157 | 34.8 | 22.1 |
| 22.2 | 295.4 | 0.494 | 0.067 | 44.6 | 9.9 |
| 27.43 | 300.58 | 0.560 | 0.000 | 52.6 | 0.0 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.
(3) Not specified.

**Estimated Error:**
Not reported.

## 5.9. Hexane+4-Methyl-cis-4-cyclohexene-1,2-dicarboxylic Anhydride

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) Hexane; $C_6H_{14}$ ; [110-54-3]
(3) 4-Methyl-cis-4-cyclohexene-1,2-dicarboxylic anhydride; $C_9H_{10}O_3$ ; [3425-89-6]

**Original Measurements:**
R. B. Snyder and C. A. Eckert, J. Chem. Eng. Data **18**, 282–5 (1973).

**Variables:**
$T$/K=306–308

**Prepared By:**
N. I. Lisov and V. P. Sazonov

**Experimental Data**

Solubility temperatures of the liquid phases

| $t$/°C | $T$/K (compilers) | $x_1$ | $x_2$ | 100 $w_1$ (compilers) | 100 $w_2$ (compilers) |
|---|---|---|---|---|---|
| 32.44 | 305.59 | 0.504 97 | 0.491 03 | 46.864 | 52.314 |
| 32.88 | 306.03 | 0.503 96 | 0.490 04 | 46.671 | 52.099 |
| 33.31 | 306.46 | 0.502 89 | 0.489 01 | 46.469 | 51.874 |
| 33.88 | 307.03 | 0.501 93 | 0.488 07 | 46.288 | 51.671 |
| 34.88 | 308.03 | 0.499 09 | 0.485 31 | 45.756 | 51.078 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solubility temperatures were determined from a set of samples made up to composition by weight and sealed into 7 mm Pyrex tubes about 9 cm long. A short length of glass rod was placed in each tube as a stirrer. An apparatus was constructed to rotate the tube end over end inside the temperature bath, so that the glass rod stirrer would fall through the liquid, causing mixing. The apparatus consisted of a submerged horizontal drive shaft with a fuse holder perpendicularly attached to one end. The sealed glass tube was placed in the fuse holder, and the shaft was rotated by a rubber pulley connected to a 4 rpm electric motor mounted on a platform above the water level.

**Source and Purity of Materials:**
(1) Distilled in 1.5 m column packed with nichrome helices; purity 99.9 mass %.
(2) Distilled at a 15:1 reflux ratio in 1 m column packed with glass helices; purity 99.9 mass %; boiling point=68.0–68.1 °C.
(3) Synthesized by the direct Diels–Alder condensation; purified by repeated recrystallization; melting point=66 °C–67 °C.

**Estimated Error:**
Temperature: control: ±0.01 K.

## 5.10. Toluene+Tricosane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Toluene; $C_7H_8$; [108-88-3]
(3) Tricosane; $C_{23}H_{48}$; [638-67-5]

**Original Measurements:**
V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (8), 9–13 (1970).

**Variables:**
$T$/K=276–334

**Prepared By:**
V. P. Sazonov and N. I. Lisov

### Experimental Data

The solubility temperatures of the liquid or solid phases were determined in ternary mixtures with a constant mass relationship of (1) and (2), respectively, 7.5:92.5, 34.5:65.5, 40.0:60.0, 71.5:28.5, and 95.0:5.0 (see Tables 1 and 2).

Table 1. Solubility temperatures of the solid phase

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship nitroethane:toluene=7.5:92.5 | | | | | |
| 3.0 | 276.2 | 7.27 | 89.85 | 0.0896 | 0.9022 |
| 11.9 | 285.1 | 6.88 | 85.03 | 0.0882 | 0.8879 |
| 18.0 | 291.2 | 6.13 | 75.87 | 0.0850 | 0.8573 |
| 22.0 | 295.2 | 5.53 | 68.27 | 0.0823 | 0.8276 |
| 25.3 | 298.5 | 4.73 | 58.47 | 0.0777 | 0.7826 |
| 32.0 | 305.2 | 3.52 | 43.38 | 0.0688 | 0.6911 |
| 39.7 | 312.9 | 2.30 | 28.30 | 0.0555 | 0.5569 |
| 44.0 | 317.2 | 1.39 | 17.11 | 0.0406 | 0.4079 |
| 46.8 | 320.0 | 0.60 | 7.32 | 0.0215 | 0.2141 |
| 48.5 | 321.7 | 0.16 | 2.04 | 0.0065 | 0.0680 |
| constant mass relationship nitroethane:toluene=34.5:65.5 | | | | | |
| 6.8 | 280.0 | 34.19 | 64.90 | 0.3917 | 0.6058 |
| 12.0 | 285.2 | 33.90 | 64.40 | 0.3907 | 0.6047 |
| 23.4 | 296.6 | 31.20 | 59.20 | 0.3821 | 0.5907 |
| 27.8 | 301.0 | 27.70 | 52.70 | 0.3685 | 0.5712 |
| 30.5 | 303.7 | 23.15 | 44.00 | 0.3476 | 0.5383 |
| 32.3 | 305.5 | 19.80 | 37.70 | 0.3281 | 0.5090 |
| 35.0 | 308.2 | 16.20 | 30.80 | 0.3025 | 0.4686 |
| 38.1 | 311.3 | 11.50 | 21.80 | 0.2574 | 0.3974 |
| 41.0 | 314.2 | 8.10 | 15.40 | 0.2113 | 0.3273 |
| 48.1 | 321.3 | 1.28 | 2.42 | 0.0502 | 0.0773 |
| constant mass relationship nitroethane:toluene=40.0:60.0 | | | | | |
| 9.2 | 282.4 | 39.72 | 59.33 | 0.4499 | 0.5476 |
| 14.7 | 287.9 | 39.24 | 58.63 | 0.4485 | 0.5459 |
| 25.3 | 298.5 | 36.20 | 54.00 | 0.4390 | 0.5335 |
| 29.2 | 302.4 | 31.60 | 47.20 | 0.4216 | 0.5130 |
| 31.1 | 304.3 | 28.50 | 42.60 | 0.4078 | 0.4966 |
| 33.2 | 306.4 | 23.90 | 35.40 | 0.3845 | 0.4640 |
| 35.0 | 308.2 | 19.90 | 29.70 | 0.3569 | 0.4340 |
| 36.0 | 309.2 | 16.70 | 24.90 | 0.3307 | 0.4018 |
| 38.8 | 312.0 | 12.60 | 18.80 | 0.2878 | 0.3499 |
| 46.5 | 319.7 | 3.95 | 5.93 | 0.1333 | 0.1631 |
| constant mass relationship nitroethane:toluene=71.5:28.5 | | | | | |
| 19.0 | 292.2 | 70.90 | 28.54 | 0.7520 | 0.2466 |
| 22.0 | 295.2 | 70.70 | 28.45 | 0.7515 | 0.2464 |
| 30.0 | 303.2 | 69.30 | 27.90 | 0.7477 | 0.2453 |
| 33.5 | 306.7 | 67.90 | 27.40 | 0.7436 | 0.2445 |
| 36.5 | 309.7 | 65.80 | 26.50 | 0.7379 | 0.2421 |
| 42.0 | 315.2 | 60.70 | 24.40 | 0.7224 | 0.2366 |
| 43.0 | 316.2 | 26.20 | 10.00 | 0.5336 | 0.1659 |
| 43.3 | 316.5 | 19.88 | 8.12 | 0.4608 | 0.1533 |
| 44.7 | 317.9 | 13.49 | 5.51 | 0.3675 | 0.1223 |
| 47.6 | 320.8 | 3.55 | 1.45 | 0.1330 | 0.0442 |
| constant mass relationship nitroethane:toluene=95.0:5.0 | | | | | |
| 37.0 | 310.2 | 94.00 | 5.10 | 0.9556 | 0.0422 |
| 42.0 | 315.2 | 93.20 | 4.98 | 0.9542 | 0.0415 |
| 45.2 | 318.4 | 92.40 | 4.96 | 0.9521 | 0.0416 |
| 45.2 | 318.4 | 91.11 | 4.59 | 0.9506 | 0.0390 |
| 45.3 | 318.5 | 89.19 | 5.69 | 0.9387 | 0.0488 |
| 45.9 | 319.1 | 19.65 | 1.25 | 0.5044 | 0.0264 |
| 46.0 | 319.2 | 21.22 | 1.36 | 0.5275 | 0.0275 |
| 46.0 | 319.2 | 17.77 | 1.13 | 0.4746 | 0.0246 |
| 46.0 | 319.2 | 6.58 | 0.42 | 0.2315 | 0.0120 |
| 49.0 | 322.2 | 0.81 | 0.05 | 0.0341 | 0.0017 |

Table 2. Solubility temperatures of the liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| constant mass relationship nitroethane:toluene=40.0:60.0 | | | | | |
| 33.5 | 306.7 | 23.90 | 35.40 | 0.3845 | 0.4640 |
| 37.5 | 310.7 | 19.90 | 29.70 | 0.3569 | 0.4340 |
| 39.1 | 312.3 | 12.60 | 18.80 | 0.2878 | 0.3499 |
| 39.8 | 313.0 | 16.70 | 24.90 | 0.3307 | 0.4018 |
| constant mass relationship nitroethane:toluene=71.5:28.5 | | | | | |
| 48.5 | 321.7 | 19.88 | 8.12 | 0.4608 | 0.1533 |
| 48.8 | 322.0 | 60.70 | 24.40 | 0.7224 | 0.2366 |
| 61.0 | 334.2 | 26.20 | 10.00 | 0.5336 | 0.1659 |
| constant mass relationship nitroethane:toluene=95.0:5.0 | | | | | |
| 46.0 | 319.2 | 92.40 | 4.96 | 0.9521 | 0.0416 |
| 50.6 | 323.8 | 19.65 | 1.25 | 0.5044 | 0.0261 |
| 58.0 | 331.2 | 91.11 | 4.59 | 0.9506 | 0.0390 |
| 60.0 | 333.2 | 21.22 | 1.36 | 0.5275 | 0.0275 |
| 60.5 | 333.7 | 89.19 | 5.69 | 0.9387 | 0.0488 |

### Auxiliary Information

**Method/Apparatus/Procedure:**
The synthetic method was used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; purified.
(3) Source not specified; purity not specified; boiling point=383.0 °C, melting point=47.7 °C.

**Estimated Error:**
Not specified.

## 5.11. Toluene+Paraffins

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) Toluene; $C_7H_8$; [108-88-3]
(3) Paraffin

**Original Measurements:**
L. M. Kozlov and V. I. Vol'pert, Tr., Kazan. Khim.-Tekhnol. Inst. **40**, 240–5 (1969).

**Variables:**
$T$/K=252–332

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**

The temperatures of phase transitions were determined in ternary mixtures with a constant mass relationship of (1) and (2) as 5.0:95.0, 10.0:90.0, 30.0:70.0, 50.0:50.0, 70.0:30.0, 80.0:20.0, 90.0:10.0, and 95.0:5.0, respectively (see Tables 1 and 2).

Table 1. Solubility temperatures of the solid phase

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ |
|---|---|---|---|
| constant mass relationship nitroethane:toluene=5.0:95.0 | | | |
| −21.5 | 251.7 | 4.95 | 94.07 |
| −18.0 | 255.2 | 4.70 | 90.24 |
| −16.0 | 257.2 | 4.22 | 85.84 |
| −12.0 | 261.2 | 3.85 | 71.15 |
| −9.5 | 263.7 | 2.97 | 51.86 |
| −2.8 | 270.4 | 2.54 | 31.72 |
| −1.0 | 272.2 | 1.56 | 27.99 |
| 1.5 | 274.7 | 1.11 | 18.83 |
| 5.0 | 278.2 | 0.43 | 9.67 |
| 8.0 | 281.2 | 0.07 | 1.82 |
| constant mass relationship nitroethane:toluene=10.0:90.0 | | | |
| −20.8 | 252.4 | 9.93 | 89.28 |
| −18.0 | 255.2 | 9.41 | 88.17 |
| −12.0 | 261.2 | 7.94 | 72.00 |
| −10.0 | 263.2 | 6.97 | 63.06 |
| −6.5 | 266.7 | 4.50 | 40.30 |
| −2.0 | 271.2 | 3.53 | 31.34 |
| 2.0 | 275.2 | 2.26 | 17.68 |
| 5.0 | 278.2 | 1.50 | 8.37 |
| 7.2 | 280.4 | 0.92 | 4.13 |
| 8.0 | 281.2 | 0.10 | 1.39 |
| constant mass relationship nitroethane:toluene=30.0:70.0 | | | |
| −20.2 | 253.0 | 30.23 | 69.17 |
| −17.0 | 256.2 | 29.00 | 67.95 |
| −14.3 | 258.9 | 27.00 | 63.98 |
| −10.0 | 263.2 | 25.16 | 57.84 |
| −6.5 | 266.7 | 19.92 | 53.23 |
| −4.0 | 269.2 | 17.98 | 44.94 |
| −0.5 | 272.7 | 14.06 | 31.88 |
| 2.0 | 275.2 | 10.04 | 21.36 |
| 3.3 | 276.5 | 5.02 | 11.86 |
| 8.0 | 281.2 | 0.54 | 1.56 |
| constant mass relationship nitroethane:toluene=50.0:50.0 | | | |
| −15.5 | 257.7 | 47.50 | 51.85 |
| −9.0 | 264.2 | 47.82 | 47.66 |
| −3.5 | 269.7 | 41.05 | 43.45 |
| −0.7 | 272.5 | 34.90 | 37.16 |
| 1.0 | 274.2 | 26.99 | 26.90 |
| 1.0 | 274.2 | 25.10 | 27.60 |
| 1.8 | 275.0 | 20.10 | 19.92 |
| 4.8 | 278.0 | 9.00 | 8.85 |
| 7.0 | 280.2 | 2.56 | 2.40 |
| 8.0 | 281.2 | 0.92 | 1.09 |
| constant mass relationship nitroethane:toluene=70.0:30.0 | | | |
| −7.5 | 265.7 | 70.42 | 28.68 |
| 2.5 | 275.7 | 60.00 | 27.91 |
| 2.5 | 275.7 | 44.85 | 20.25 |
| 3.5 | 276.7 | 39.98 | 17.60 |
| 4.5 | 277.7 | 25.20 | 10.82 |
| 5.3 | 278.5 | 20.05 | 9.83 |
| 6.8 | 280.0 | 13.95 | 5.97 |
| 7.5 | 280.7 | 9.93 | 3.84 |
| 8.0 | 281.2 | 2.70 | 1.29 |
| 8.0 | 281.2 | 1.68 | 0.72 |
| constant mass relationship nitroethane:toluene=80.0:20.0 | | | |
| −0.5 | 272.7 | 79.50 | 19.61 |
| 4.5 | 277.7 | 75.13 | 19.74 |
| 4.5 | 277.7 | 70.10 | 16.94 |
| 4.8 | 278.0 | 65.58 | 15.37 |
| 5.0 | 278.2 | 50.00 | 12.92 |
| 6.0 | 279.2 | 19.95 | 5.05 |
| 7.5 | 280.7 | 15.09 | 4.91 |
| 8.0 | 281.2 | 9.85 | 3.08 |
| 8.3 | 281.5 | 6.09 | 1.92 |
| 8.3 | 281.5 | 2.46 | 0.54 |
| constant mass relationship nitroethane:toluene=90.0:10.0 | | | |
| 3.0 | 276.2 | 90.07 | 8.27 |
| 5.0 | 278.2 | 84.92 | 9.95 |
| 6.0 | 279.2 | 76.10 | 15.25 |
| 6.0 | 279.2 | 74.80 | 10.10 |
| 7.3 | 280.5 | 18.46 | 1.51 |
| 8.2 | 281.4 | 14.92 | 1.38 |
| 8.2 | 281.4 | 11.04 | 1.27 |
| 8.2 | 281.4 | 9.05 | 0.90 |
| 8.2 | 281.4 | 6.00 | 1.05 |
| 8.5 | 281.7 | 1.80 | 0.26 |
| constant mass relationship nitroethane:toluene=95.0:5.0 | | | |
| 4.0 | 277.7 | 94.98 | 4.35 |
| 8.0 | 281.2 | 90.46 | 4.48 |
| 8.0 | 281.2 | 84.93 | 6.12 |
| 8.0 | 281.2 | 79.98 | 5.07 |
| 8.2 | 281.4 | 14.99 | 1.05 |
| 8.2 | 281.4 | 9.95 | 1.07 |
| 8.2 | 281.4 | 6.50 | 0.44 |
| 8.5 | 281.7 | 2.53 | 0.47 |
| 8.5 | 281.7 | 1.28 | 0.46 |
| 8.8 | 282.0 | 0.24 | 0.20 |

Table 2. Solubility temperatures of the liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ |
|---|---|---|---|
| | constant mass relationship nitroethane:toluene=50.0:50.0 | | |
| 13 | 286.2 | 25.10 | 27.60 |
| 16 | 289.2 | 26.99 | 26.90 |
| 22 | 295.2 | 9.00 | 8.85 |
| 24 | 297.2 | 20.10 | 19.92 |
| 31 | 304.2 | 9.93 | 3.84 |
| 36 | 309.2 | 44.85 | 20.25 |
| 40 | 313.2 | 39.98 | 17.60 |
| 42 | 315.2 | 13.95 | 5.97 |
| 46 | 319.2 | 20.05 | 9.83 |
| 48 | 321.2 | 25.20 | 10.82 |
| | constant mass relationship nitroethane:toluene=80.0:20.0 | | |
| 11 | 284.2 | 6.09 | 1.92 |
| 32 | 305.2 | 9.85 | 3.08 |
| 36 | 309.2 | 70.10 | 16.94 |
| 46 | 319.2 | 65.58 | 15.37 |
| 48 | 321.2 | 15.09 | 4.91 |
| 48 | 321.2 | 19.95 | 5.05 |
| 54 | 327.2 | 50.00 | 12.92 |
| | constant mass relationship nitroethane:toluene=90.0:10.0 | | |
| 25 | 298.2 | 84.92 | 9.95 |
| 30 | 303.2 | 76.10 | 15.25 |
| 30 | 303.2 | 11.04 | 1.27 |
| 32 | 305.2 | 14.92 | 1.38 |
| 49 | 322.2 | 74.80 | 10.10 |
| 55 | 328.2 | 18.46 | 1.51 |
| | constant mass relationship nitroethane:toluene=95.0:5.0 | | |
| 32 | 305.2 | 90.46 | 4.48 |
| 37 | 310.2 | 9.95 | 1.07 |
| 48.5 | 321.7 | 14.99 | 1.05 |
| 52 | 325.2 | 84.93 | 6.12 |
| 59 | 332.2 | 79.98 | 5.07 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used.
No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.
(3) Narrow fraction of liquid paraffin separated in the interval of 195 °C–270 °C is treated by urea; melting point=9 °C.

**Estimated Error:**
Not specified.

## 5.12. 1-Octene+Octane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Octene; $C_8H_{16}$; [111-66-0]
(3) Octane; $C_8H_{18}$; [111-65-9]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K=273

**Prepared By:**
V. P. Sazonov

**Experimental Data**

Table 1. Mutual solubility of nitroethane (1), 1-octene (2) and octane (3)

| $t$/°C | $T$/K (compiler) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compiler) | $x_2$ (compiler) |
|---|---|---|---|---|---|
| 0.0 | 273.2 | 7.7 | 20.5 | 0.112 | 0.200 |
| | | 15.2 | 57.9 | 0.212 | 0.541 |
| | | 17.4 | 59.3 | 0.240 | 0.548 |
| | | 24.0 | 60.5 | 0.321 | 0.542 |
| | | 29.1 | 60.2 | 0.381 | 0.527 |
| | | 34.0 | 58.2 | 0.436 | 0.499 |
| | | 50.6 | 44.9 | 0.605 | 0.359 |
| | | 52.9 | 43.0 | 0.627 | 0.341 |
| | | 74.7 | 20.5 | 0.816 | 0.150 |
| | | 80.6 | 13.7 | 0.862 | 0.098 |
| | | 83.2 | 10.2 | 0.882 | 0.072 |

Table 2. Composition of the equilibrium liquid phases

| | | Nitroethane-rich phase | | Hydrocarbon-rich phase | | Nitroethane-rich phase (compiler) | | Hydrocarbon-rich phase (compiler) | |
|---|---|---|---|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1'$ | 100 $w_2'$ | 100 $w_1''$ | 100 $w_2''$ | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ |
| 0.0 | 273.2 | 88.6 | 3.1 | 7.9 | 25.3 | 0.922 | 0.021 | 0.115 | 0.246 |
| | | 85.2 | 7.8 | 9.9 | 38.6 | 0.897 | 0.055 | 0.142 | 0.371 |
| | | 81.2 | 12.3 | 12.9 | 50.3 | 0.866 | 0.088 | 0.178 | 0.476 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Two methods were used. The cloud point was determined by titrating a third component into binary samples of known composition in a constant temperature bath. In the given system no distinct change in the transparency of the clear mixture was observed to indicate to the unaided eye that the cloud point had been obtained; only the, presence of finely dispersed globules of the second phase, which were visible through a magnifying glass denoted the fact that the cloud point had been reached. The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques (see Tables 1 and 2).

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.
(3) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: ±0.05 K.

## 5.13. 2,2,4-Trimethylpentane+Octane

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]
(3) Octane; $C_8H_{18}$ ; [111-65-9]

**Original Measurements:**
S. C. P. Hwa, R. Techo, and W. T. Ziegler, J. Chem. Eng. Data **8**, 409–11 (1963).

**Variables:**
$T$/K=298 and 308

**Prepared By:**
V. P. Sazonov

**Experimental Data**

Table 1. Mutual solubility of nitroethane (1), 2,2,4-trimethylpentane (2) and octane (3)

| $t$/°C | $T$/K (compiler) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compiler) | $x_2$ (compiler) |
|---|---|---|---|---|---|
| 35.0 | 308.2 | 26.2 | 23.5 | 0.351 | 0.207 |
| | | 27.0 | 25.0 | 0.360 | 0.219 |
| | | 40.5 | 37.4 | 0.509 | 0.309 |
| | | 56.8 | 26.5 | 0.667 | 0.204 |
| | | 59.1 | 24.0 | 0.687 | 0.183 |
| | | 71.8 | 4.5 | 0.795 | 0.033 |

Table 2. Composition of equilibrium liquid phases

| | | Nitroethane-rich phase | | Hydrocarbon-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1'$ | 100 $w_2'$ | 100 $w_1''$ | 100 $w_2''$ |
| 25.0 | 298.2 | 82.6 | 1.7 | 13.7 | 7.7 |
| | | 79.7 | 8.3 | 14.9 | 33.2 |
| | | 76.4 | 15.1 | 16.8 | 49.8 |
| 35.0 | 308.2 | 72.1 | 4.6 | 26.0 | 12.1 |
| | | 69.9 | 8.4 | 26.3 | 20.9 |
| | | 63.7 | 17.9 | 30.1 | 35.2 |
| | | 62.1 | 20.7 | 31.9 | 36.2 |

The same data are presented below in mole fractions

| | | Nitroethane-rich phase (compiler) | | Hydrocarbon-rich phase (compiler) | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ |
| 25.0 | 298.2 | 0.878 | 0.012 | 0.195 | 0.072 |
| | | 0.857 | 0.059 | 0.210 | 0.308 |
| | | 0.831 | 0.108 | 0.235 | 0.458 |
| 35.0 | 308.2 | 0.797 | 0.033 | 0.348 | 0.107 |
| | | 0.779 | 0.062 | 0.352 | 0.184 |
| | | 0.728 | 0.134 | 0.396 | 0.304 |
| | | 0.714 | 0.156 | 0.416 | 0.310 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Two methods were used. The cloud point was determined by titrating a third component into binary samples of known composition in a constant temperature bath. In the given system no distinct change in the transparency of the clear mixture was observed to indicate to the unaided eye that the cloud point had been obtained; only the presence of finely dispersed globules of the second phase, which were visible through a magnifying glass, denoted the fact that the cloud point had been reached. The analytical method consisted of withdrawing a sample from each of the coexisting phases from an equilibrium cell in a constant temperature bath, and analyzing the samples by gas chromatographic techniques.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; purity 96 mole % with 3.9 mole % of 2-nitropropane; not purified.
(2) Phillips Petroleum Co.; purity >99 mole %; not purified.
(3) Phillips Petroleum Co.; purity >99 mole %; not purified.

**Estimated Error:**
Temperature: ±0.05 K.

## 5.14. 2,2,4-Trimethylpentane+Heptacosafluorotributanamine

**Components:**
(1) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(2) 2,2,4-Trimethylpentane; $C_8H_{18}$ ; [540-84-1]
(3) Heptacosafluorotributanamine; $C_{12}F_{27}N$; [311-89-7]

**Original Measurements:**
J. Vreeland and R. Dunlap, J. Phys. Chem. **61**, 329–33 (1957).

**Variables:**
$T$/K=298–325

**Prepared By:**
V. P. Sazonov, N. I. Lisov, and N. V. Sazonov

**Experimental Data**

Table 1. Mutual solubility of nitroethane (1), 2,2,4-trimethylpentane (2) and Heptacosafluorotributanamine (3)[a]

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 25.0 | 298.2 | 22.2 | 77.8 | 0.303 | 0.697 |
| | | 67.7 | 32.3 | 0.761 | 0.239 |
| | | 4.0 | 81.8 | 0.067 | 0.906 |
| | | 13.4 | 75.5 | 0.209 | 0.772 |
| | | 16.4 | 73.6 | 0.249 | 0.734 |
| | | 18.8 | 76.2 | 0.271 | 0.721 |
| | | 69.0 | 30.0 | 0.777 | 0.222 |
| | | 75.0 | 23.6 | 0.827 | 0.171 |
| | | 2.5 | 5.0 | 0.155 | 0.204 |
| | | 2.2 | 7.8 | 0.126 | 0.295 |
| | | 0.0 | 7.6 | 0.0 | 0.326 |
| | | 0.0 | 83.5 | 0.0 | 0.968 |
| | | 0.1 | 0.0 | 0.009 | 0.0 |
| | | 99.9 | 0.0 | 0.999 | 0.0 |
| | | 20.9* | 12.6* | 0.571 | 0.226 |
| | | 37.1* | 16.8* | 0.696 | 0.207 |
| | | 46.0* | 19.4* | 0.734 | 0.204 |
| | | 60.9* | 23.6* | 0.779 | 0.199 |
| | | 5.0* | 15.0* | 0.210 | 0.414 |
| | | 7.9* | 28.8* | 0.233 | 0.558 |
| | | 11.7* | 47.2* | 0.247 | 0.656 |
| | | 15.4* | 70.5* | 0.243 | 0.732 |
| | | 19.6* | 69.9* | 0.294 | 0.689 |
| | | 46.7* | 47.0* | 0.596 | 0.395 |
| 31.5 | 304.7 | 5.0 | 75.0 | 0.088 | 0.872 |
| | | 15.0 | 67.8 | 0.244 | 0.725 |
| | | 1.3 | 12.6 | 0.068 | 0.431 |
| | | 30.0 | 60.6 | 0.423 | 0.562 |
| | | 42.2 | 51.3 | 0.550 | 0.440 |
| | | 58.8 | 37.6 | 0.701 | 0.294 |
| | | 75.0 | 22.4 | 0.833 | 0.164 |
| | | 85.0 | 13.9 | 0.902 | 0.097 |
| | | 2.0 | 10.0 | 0.108 | 0.357 |
| | | 0.0 | 8.8 | 0.0 | 0.362 |
| | | 0.0 | 77.6 | 0.0 | 0.953 |
| | | 0.1 | 0.0 | 0.009 | 0.0 |
| | | 99.9 | 0.0 | 0.999 | 0.0 |
| | | 8.1* | 26.5* | 0.247 | 0.530 |
| | | 13.1* | 39.6* | 0.295 | 0.586 |
| | | 17.4* | 52.1* | 0.316 | 0.622 |
| | | 29.8* | 58.5* | 0.428 | 0.553 |
| | | 40.0* | 50.0* | 0.541 | 0.444 |
| | | 57.3* | 36.6* | 0.699 | 0.293 |
| | | 10.0* | 14.5* | 0.357 | 0.341 |
| | | 30.0* | 20.0* | 0.615 | 0.270 |
| | | 50.0* | 25.0* | 0.722 | 0.237 |
| 33.7 | 306.9 | 7.1 | 71.4 | 0.126 | 0.832 |
| | | 20.0 | 63.1 | 0.316 | 0.654 |
| | | 30.0 | 58.4 | 0.430 | 0.551 |
| | | 2.2 | 9.5 | 0.120 | 0.341 |
| | | 41.6 | 52.3 | 0.543 | 0.448 |
| | | 48.3 | 46.3 | 0.609 | 0.383 |
| | | 53.6 | 41.2 | 0.660 | 0.333 |
| | | 60.0 | 35.9 | 0.714 | 0.281 |
| | | 77.0 | 24.3 | 0.830 | 0.172 |
| | | 80.8 | 14.0 | 0.892 | 0.102 |
| | | 1.9 | 5.1 | 0.121 | 0.214 |
| | | 0.0 | 10.1 | 0.0 | 0.398 |
| | | 0.0 | 75.0 | 0.0 | 0.946 |
| | | 0.1 | 0.0 | 0.009 | 0.0 |
| | | 99.9 | 0.0 | 0.999 | 0.0 |
| | | 11.1* | 14.1* | 0.386 | 0.323 |
| | | 17.9* | 30.9* | 0.407 | 0.462 |
| | | 27.6* | 48.6* | 0.444 | 0.513 |
| | | 32.3* | 54.1* | 0.466 | 0.512 |
| | | 12.1* | 14.1* | 0.408 | 0.313 |
| | | 20.8* | 18.9* | 0.520 | 0.311 |
| | | 37.7* | 29.1* | 0.623 | 0.316 |
| | | 46.8* | 34.0* | 0.656 | 0.313 |
| | | 40.7* | 51.7* | 0.539 | 0.450 |
| | | 47.3* | 45.6* | 0.606 | 0.384 |
| | | 52.7* | 41.1* | 0.655 | 0.336 |
| 35.0 | 308.2 | 7.1 | 68.1 | 0.130 | 0.819 |
| | | 20.0 | 62.0 | 0.319 | 0.649 |
| | | 28.8 | 57.1 | 0.424 | 0.553 |
| | | 35.0 | 53.8 | 0.489 | 0.494 |
| | | 40.0 | 51.0 | 0.537 | 0.450 |
| | | 57.3 | 37.1 | 0.696 | 0.296 |
| | | 62.9 | 33.3 | 0.738 | 0.257 |
| | | 72.1 | 25.2 | 0.810 | 0.186 |
| | | 85.0 | 13.5 | 0.904 | 0.094 |
| | | 1.6 | 8.4 | 0.093 | 0.321 |
| | | 2.6 | 5.1 | 0.160 | 0.206 |
| | | 0.0 | 10.6 | 0.0 | 0.411 |
| | | 0.0 | 74.1 | 0.0 | 0.944 |
| | | 0.1 | 0.0 | 0.009 | 0.0 |
| | | 99.9 | 0.0 | 0.999 | 0.0 |
| 51.3 | 324.5 | 2.0 | 8.3 | 0.114 | 0.312 |
| | | 3.0 | 17.4 | 0.128 | 0.490 |
| | | 5.0 | 30.0 | 0.156 | 0.616 |
| | | 8.8 | 41.2 | 0.212 | 0.653 |
| | | 14.6 | 50.0 | 0.284 | 0.639 |
| | | 30.0 | 50.0 | 0.461 | 0.505 |
| | | 43.9 | 43.8 | 0.593 | 0.389 |
| | | 50.0 | 40.0 | 0.646 | 0.340 |
| | | 61.8 | 32.2 | 0.739 | 0.253 |
| | | 70.0 | 26.6 | 0.797 | 0.199 |
| | | 83.4 | 14.7 | 0.894 | 0.104 |
| | | 0.1 | 0.0 | 0.009 | 0.0 |
| | | 99.9 | 0.0 | 0.999 | 0.0 |

[a]These data were extracted from published graphs by the compilers.
*Values marked with asterisks correspond to composition of ternary mixtures with transition of the equilibrium of two liquid phases in equilibrium of the three liquid phases.

Table 2. Compositions of the three equilibrium liquid phases

| $t$/°C | $T$/K (compilers) | Amine-rich phase 100 $w_1'$ | Amine-rich phase 100 $w_2'$ | Hydrocarbon-rich phase 100 $w_1''$ | Hydrocarbon-rich phase 100 $w_2''$ | Nitroethane-rich phase 100 $w_1'''$ | Nitroethane-rich phase 100 $w_2'''$ |
|---|---|---|---|---|---|---|---|
| 25.0 | 298.2 | 4.2 | 7.5 | 15.9 | 72.2 | 71.2 | 26.9 |
| 31.5 | 304.7 | 2.8 | 12.4 | 22.1 | 64.2 | 67.6 | 29.5 |
| 33.7 | 306.9 | 3.5 | 8.7 | 33.6 | 57.5 | 55.5 | 39.6 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Amine-rich phase (compilers) $x_1'$ | Amine-rich phase (compilers) $x_2'$ | Hydrocarbon-rich phase (compilers) $x_1''$ | Hydrocarbon-rich phase (compilers) $x_2''$ | Nitroethane-rich phase (compilers) $x_1'''$ | Nitroethane-rich phase (compilers) $x_2'''$ |
|---|---|---|---|---|---|---|---|
| 25.0 | 298.2 | 0.221 | 0.259 | 0.246 | 0.734 | 0.799 | 0.198 |
| 31.5 | 304.7 | 0.137 | 0.399 | 0.336 | 0.641 | 0.774 | 0.222 |
| 33.7 | 306.9 | 0.184 | 0.300 | 0.464 | 0.522 | 0.676 | 0.317 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The titration method was used. The third component was added until a phase just disappeared or reappeared. These titrations were carried out in stoppered 150 mm test tubes which (were placed) in temperature baths. In cases where a shift from two phases to one was approached, the size of one layer usually decreased faster than the other upon addition of the third component. When such behavior was observed, addition of the third component was made dropwise until the system became homogeneous. Near the end point, 10 min were allowed between drops in order to establish temperature equilibrium. In cases requiring a shift from two to three phases, it was found difficult to observe the appearance of the third phase when it appeared at the interface or the meniscus. In such cases, making up a three-phase solution and titrating with a third component until the shift from three to two phases was observed obtained greater reproducibility.

**Source and Purity of Materials:**

(1) Matheson Chemical Co.; research grade; distilled through a Todd column; boiling point=114.7 °C–114.8 °C.
(2) Phillips Petroleum Co.; pure grade; 99 mole % minimum; $\rho$(25 °C)=687.74 g·L$^{-1}$, not purified.
(3) Minnesota Mining and Manufacturing Co.; distilled through a Todd column; boiling point=178.0 °C–178.1 °C.

**Estimated Error:**

Temperature: ±0.05 K, composition: 1%;
Titer: ±0.002 mL.

# 6. Multicomponent Systems with Nitroethane

## 6.1. Methanol+1,2-Ethanediol+Cyclohexane

**Components:**

(1) Methanol; $CH_4O$; [67-56-1]
(2) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(3) 1.2-Ethanediol; $C_2H_6O_2$; [107-21-1]
(4) Cyclohexane; $C_6H_{12}$; [110-82-7]

**Original Measurements:**

J. Chrapec, S. Rzoska, and J. Ziolo, Phase Transitions **4**, 73–80 (1983).

**Variables:**

$T$/K=296–307

**Prepared By:**

V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The solubility temperatures of liquid phases were determined in quaternary mixtures with a constant mass relationship of (1), (2), and (3), and also in quaternary mixtures with a constant mass relationship of (1), (2), and (4).

Solubility temperatures of the three liquid phases

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | 100 $w_3$ | $x_1$ (compilers) | $x_2$ (compilers) | $x_3$ (compilers) |
|---|---|---|---|---|---|---|---|
| constant mass relationship methanol:nitroethane:1,2-ethanediol=7.0:64.2:28.8 | | | | | | | |
| 23.3 | 296.5 | 5.3 | 48.8 | 21.9 | 0.114 | 0.447 | 0.243 |
| 24.3 | 297.5 | 5.0 | 46.2 | 20.8 | 0.108 | 0.428 | 0.233 |
| 24.9 | 298.1 | 3.2 | 29.5 | 13.3 | 0.074 | 0.291 | 0.159 |
| 25.4 | 298.6 | 4.7 | 42.8 | 19.2 | 0.103 | 0.401 | 0.218 |
| 25.5 | 298.7 | 3.7 | 33.6 | 15.1 | 0.084 | 0.326 | 0.177 |
| 25.7 | 298.9 | 4.0 | 36.9 | 16.6 | 0.090 | 0.354 | 0.193 |
| 25.8 | 299.0 | 4.4 | 40.0 | 18.0 | 0.098 | 0.379 | 0.206 |
| constant mass relationship methanol:nitroethane:1,2-ethanediol=9.5:62.4:28.1 | | | | | | | |
| 24.3 | 297.5 | 3.1 | 20.1 | 9.0 | 0.074 | 0.204 | 0.110 |
| 24.9 | 298.1 | 7.2 | 47.4 | 21.4 | 0.151 | 0.425 | 0.232 |
| 25.8 | 299.0 | 3.5 | 22.8 | 10.2 | 0.082 | 0.228 | 0.123 |
| 26.8 | 300.0 | 6.9 | 45.0 | 20.3 | 0.146 | 0.407 | 0.222 |
| 27.0 | 300.2 | 3.8 | 25.0 | 11.2 | 0.088 | 0.248 | 0.134 |
| 28.1 | 301.3 | 6.4 | 41.8 | 18.8 | 0.138 | 0.384 | 0.209 |
| 28.2 | 301.4 | 4.5 | 29.3 | 13.2 | 0.102 | 0.284 | 0.155 |
| 28.6 | 301.8 | 4.9 | 32.5 | 14.6 | 0.110 | 0.311 | 0.169 |
| 28.7 | 301.9 | 5.9 | 38.7 | 17.4 | 0.129 | 0.360 | 0.196 |
| 28.7 | 301.9 | 5.4 | 35.6 | 16.0 | 0.119 | 0.336 | 0.183 |
| constant mass relationship methanol:nitroethane:1,2-ethanediol=11.0:61.4:27.6 | | | | | | | |
| 24.5 | 297.7 | 4.0 | 22.4 | 10.1 | 0.093 | 0.223 | 0.121 |
| 26.1 | 299.3 | 8.5 | 47.6 | 21.4 | 0.176 | 0.419 | 0.228 |
| 26.8 | 300.0 | 4.7 | 26.4 | 11.9 | 0.107 | 0.257 | 0.140 |
| 27.7 | 300.9 | 8.3 | 46.0 | 20.7 | 0.172 | 0.409 | 0.222 |
| 28.1 | 301.3 | 5.3 | 29.3 | 13.2 | 0.119 | 0.281 | 0.153 |
| 28.8 | 302.0 | 7.8 | 43.8 | 19.7 | 0.164 | 0.393 | 0.214 |
| 29.1 | 302.3 | 5.8 | 32.6 | 14.6 | 0.129 | 0.308 | 0.167 |
| 29.3 | 302.6 | 6.3 | 35.0 | 15.7 | 0.138 | 0.327 | 0.177 |
| 29.4 | 302.6 | 7.3 | 40.8 | 18.4 | 0.155 | 0.371 | 0.202 |
| 29.6 | 302.8 | 6.8 | 38.2 | 17.2 | 0.147 | 0.352 | 0.191 |
| constant mass relationship methanol:nitroethane:1,2-ethanediol=12.0:60.7:27.3 | | | | | | | |
| 26.0 | 299.2 | 5.1 | 25.8 | 11.6 | 0.116 | 0.250 | 0.136 |
| 27.0 | 300.2 | 9.6 | 48.6 | 21.8 | 0.195 | 0.422 | 0.229 |
| 27.6 | 300.8 | 5.7 | 28.7 | 12.9 | 0.128 | 0.274 | 0.149 |
| 29.5 | 302.7 | 6.3 | 32.1 | 14.4 | 0.139 | 0.302 | 0.164 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 29.8 | 303.0 | 9.1 | 45.8 | 20.6 | 0.187 | 0.402 | 0.219 |
| 30.5 | 303.7 | 7.0 | 35.2 | 15.8 | 0.152 | 0.325 | 0.177 |
| 30.8 | 304.0 | 8.6 | 43.7 | 19.7 | 0.179 | 0.388 | 0.211 |
| 31.2 | 304.4 | 7.6 | 38.5 | 17.3 | 0.162 | 0.350 | 0.190 |
| 31.3 | 304.5 | 8.0 | 40.4 | 18.1 | 0.169 | 0.364 | 0.197 |
| constant mass relationship methanol:nitroethane:1,2-ethanediol=13.0:60.0:27.0 | | | | | | | |
| 24.9 | 298.1 | 5.6 | 25.8 | 11.6 | 0.126 | 0.249 | 0.135 |
| 26.8 | 300.0 | 6.2 | 28.8 | 13.0 | 0.138 | 0.273 | 0.149 |
| 29.5 | 302.7 | 10.4 | 48.0 | 21.6 | 0.209 | 0.413 | 0.225 |
| 29.9 | 303.1 | 7.4 | 34.2 | 15.4 | 0.160 | 0.315 | 0.172 |
| 31.2 | 304.4 | 8.1 | 37.2 | 16.7 | 0.172 | 0.337 | 0.183 |
| 31.4 | 304.6 | 9.9 | 45.6 | 20.5 | 0.202 | 0.396 | 0.216 |
| 32.2 | 305.4 | 8.7 | 40.2 | 18.1 | 0.182 | 0.359 | 0.196 |
| 32.4 | 305.6 | 9.4 | 43.2 | 19.4 | 0.194 | 0.380 | 0.206 |
| constant mass relationship methanol:nitroethane:1,2-ethanediol=13.2:59.9:26.9 | | | | | | | |
| 31.0 | 304.2 | 10.6 | 47.9 | 21.5 | 0.213 | 0.411 | 0.223 |
| 31.9 | 305.1 | 8.3 | 37.4 | 16.8 | 0.176 | 0.338 | 0.184 |
| 32.4 | 305.6 | 10.4 | 47.0 | 21.1 | 0.210 | 0.405 | 0.220 |
| 33.2 | 306.4 | 8.9 | 40.1 | 18.0 | 0.186 | 0.358 | 0.194 |
| 33.8 | 307.0 | 9.9 | 44.9 | 20.2 | 0.202 | 0.391 | 0.213 |
| 33.8 | 307.0 | 9.2 | 41.6 | 18.7 | 0.191 | 0.368 | 0.200 |
| 34.0 | 307.2 | 9.4 | 42.5 | 19.1 | 0.194 | 0.375 | 0.204 |

Estimated tricritical point of quaternary system is 37.5±1 °C at $x_1=0.45$, $x_2=0.06$, $x_3=0.09$, and $x_4=0.45$ ($100\,w_1=45.1$, $100\,w_2=2.6$, $100\,w_3=7.5$, and $100\,w_4=44.9$, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solutions were placed in closed glass ampoules. The temperature at which the second meniscus appeared was estimated visually. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.
(3) Not specified.
(4) Not specified.

**Estimated Error:**
Temperature: ±0.1 K.

## 6.2. 1-Nitropropane+2-Nitropropane+Oil Fraction of Tuimazin Crude

**Components:**
(1) Nitroethane; $C_2H_5NO_2$; [79-24-3]
(2) 1-Nitropropane; $C_3H_7NO_2$; [108-03-2]
(3) 2-Nitropropane; $C_3H_7NO_2$; [79-46-9]
(4) Oil fraction of Tuimazin crude

**Original Measurements:**
V. V. Pol'shinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9–13 (1970).

**Variables:**
$T$/K=255–334

**Prepared By:**
V. P. Sazonov and N. I. Lisov

**Experimental Data**
Values of critical solution temperatures of mixed nitroparaffins (1)–(3) and stocks of fractions of Tuimazin crude (2) were presented in graphical form over the temperature range.

Mean values of critical solution temperatures of mixture nitroparaffins (1)–(3) and stocks of oil fraction of Tuimazin crude (2)

| Stock of oil fraction | $d$(20 °C,4 °C) | $n$(20 °C,D) | $T$/°C | $T$/K (compiler) |
|---|---|---|---|---|
| Heavily aromatics | 1.0232–1.0479 | 1.5787–1.5979 | −18.5 | 254.7 |
| Mean aromatics | 0.9706–0.9921 | 1.5430–1.5623 | −3.5 | 269.7 |
| Light aromatics | 0.9176 | 1.5090 | 21.5 | 294.7 |
| Paraffin–naphthenes | 0.8195–0.8667 | 1.4320*–1.4756 | 61.0 | 334.2 |

*$n$(70 °C,D)

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Bondarev and Kozlov[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1)–(3) obtained by nitration gas distillate; contained 23 vol. % nitroethane, 48.7 vol. % 1-nitropropane and 28.3 vol. % 2-nitropropane; $n$(20 °C,D)=1.3975; $d$(20 °C,4 °C)=1.0088.
(4) Obtained by distillation of Tuimazin crude between 440 and 520 °C; stocks obtained by division of oil fraction on silica gel by liquid chromatography.

**Estimated Error:**
Not specified.

**References:**
[1]S. V. Bondarev and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 10 (1970).

## 6.3. Nitromethane+1,2-Ethanediol+1-Dodecanol+Water

**Components:**

(1) Nitromethane; $CH_3NO_2$ ; [75-52-5]
(2) Nitroethane; $C_2H_5NO_2$ ; [79-24-3]
(3) 1,2-Ethanediol; $C_2H_6O_2$ ; [107-21-1]
(4) 1-Dodecanol; $C_{12}H_{26}O$; [112-53-8]
(5) Water; $H_2O$; [7732-18-5]

**Original Measurements:**

B. K. Das and R. B. Griffiths, J. Chem. Phys. **70**, 5555–66 (1979).

**Variables:**

$T$/K=311–315

**Prepared By:**

N. I. Lisov and V. P. Sazonov

**Experimental Data**

The usual order of the four phases in the sample tube. $L_1$-upper liquid phase, $L_2$-second from the top liquid phase, $L_3$-second from the bottom liquid phase, $L_4$-lower liquid phase.

Compositions of the four equilibrium liquid phases

| $t$/°C | $T$/K (compilers) | Phase | 100 $w_1$ | 100 $w_2$ | 100 $w_3$ | 100 $w_4$ |
|---|---|---|---|---|---|---|
| 37.58 | 310.73 | $L_1$ | 31.4 | 4.3 | 32.0 | 29.4 |
| | | $L_2$ | 31.5 | 3.9 | 41.6 | 18.5 |
| | | $L_3$ | 56.9 | 7.4 | 21.1 | 12.6 |
| | | $L_4$ | 30.3 | 3.8 | 48.1 | 12.7 |
| 37.92 | 311.07 | $L_1$ | 30.5 | 4.4 | 30.6 | 31.8 |
| | | $L_2$ | 45.9 | 6.4 | 30.0 | 15.0 |
| | | $L_3$ | 55.4 | 7.2 | 22.5 | 12.7 |
| | | $L_4$ | 29.5 | 3.6 | 50.0 | 11.3 |
| 38.55 | 311.70 | $L_1$ | 33.7 | 3.9 | 26.8 | 32.4 |
| | | $L_2$ | 34.9 | 3.7 | 34.9 | 22.0 |
| | | $L_3$ | 63.3 | 6.9 | 18.8 | 8.4 |
| | | $L_4$ | 33.2 | 3.4 | 48.6 | 8.3 |
| 38.84 | 311.99 | $L_1$ | 28.0 | 3.9 | 27.4 | 37.7 |
| | | $L_2$ | 35.9 | 4.6 | 33.2 | 22.7 |
| | | $L_3$ | 54.7 | 6.6 | 22.8 | 13.3 |
| | | $L_4$ | 27.5 | 2.8 | 54.4 | 8.6 |
| 39.01 | 312.16 | $L_1$ | 33.8 | 2.9 | 30.2 | 29.2 |
| | | $L_2$ | 37.0 | 2.8 | 39.3 | 15.5 |
| | | $L_3$ | 61.1 | 5.1 | 20.2 | 11.0 |
| | | $L_4$ | 34.6 | 2.5 | 46.9 | 9.3 |
| 39.26 | 312.41 | $L_1$ | 32.2 | 2.7 | 31.5 | 29.5 |
| | | $L_2$ | 33.9 | 2.6 | 36.5 | 22.4 |
| | | $L_3$ | 58.4 | 4.6 | 21.1 | 13.1 |
| | | $L_4$ | 32.0 | 2.5 | 49.0 | 10.2 |
| 39.39 | 312.54 | $L_1$ | 32.4 | 4.1 | 27.9 | 33.1 |
| | | $L_2$ | 40.9 | 4.8 | 29.2 | 22.2 |
| | | $L_3$ | 53.7 | 6.0 | 23.4 | 14.5 |
| | | $L_4$ | 28.9 | 2.7 | 54.5 | 6.9 |
| 39.40 | 312.55 | $L_1$ | 37.2 | 3.7 | 31.8 | 23.4 |
| | | $L_2$ | 37.0 | 3.6 | 35.6 | 19.4 |
| | | $L_3$ | 55.8 | 5.5 | 22.1 | 13.9 |
| | | $L_4$ | 29.4 | 2.5 | 53.9 | 7.0 |
| 39.50 | 312.65 | $L_1$ | 36.3 | 3.6 | 26.7 | 30.0 |
| | | $L_2$ | 38.2 | 3.6 | 33.3 | 20.6 |
| | | $L_3$ | 58.0 | 5.6 | 21.1 | 12.6 |
| | | $L_4$ | 30.2 | 2.3 | 53.8 | 6.2 |
| 39.76 | 312.91 | $L_1$ | 26.7 | 2.5 | 25.0 | 42.4 |
| | | $L_2$ | 35.5 | 3.0 | 37.0 | 19.6 |
| | | $L_3$ | 55.2 | 4.5 | 22.5 | 14.7 |
| | | $L_4$ | 29.7 | 2.5 | 45.7 | 15.6 |
| 39.97 | 313.12 | $L_1$ | 30.8 | 2.3 | 25.3 | 38.3 |
| | | $L_2$ | 38.4 | 2.5 | 38.8 | 14.7 |
| | | $L_3$ | 60.4 | 3.9 | 21.2 | 11.5 |
| | | $L_4$ | 36.4 | 2.3 | 44.2 | 9.9 |
| 40.02 | 313.17 | $L_1$ | 31.2 | 2.6 | 46.4 | 25.8 |
| | | $L_2$ | 35.9 | 2.8 | 36.0 | 19.8 |
| | | $L_3$ | 54.2 | 4.2 | 25.6 | 13.0 |
| | | $L_4$ | 29.7 | 2.0 | 53.1 | 6.9 |
| 40.08 | 313.23 | $L_1$ | 20.2 | 1.5 | 27.2 | 45.0 |
| | | $L_2$ | 44.6 | 2.1 | 37.3 | 17.4 |
| | | $L_3$ | 52.3 | 2.5 | 22.4 | 13.9 |
| | | $L_4$ | 31.7 | 1.5 | 50.0 | 5.1 |
| 40.15 | 313.30 | $L_1$ | 32.1 | 2.2 | 24.3 | 35.2 |
| | | $L_2$ | 40.7 | 2.3 | 36.0 | 14.5 |
| | | $L_3$ | 59.2 | 3.6 | 22.1 | 11.6 |
| | | $L_4$ | 32.8 | 1.6 | 40.0 | 8.2 |
| 40.28 | 313.43 | $L_1$ | 31.5 | 2.2 | 30.7 | 38.4 |
| | | $L_2$ | 41.1 | 2.5 | 31.2 | 15.3 |
| | | $L_3$ | 59.2 | 4.0 | 27.4 | 11.5 |
| | | $L_4$ | 42.3 | 2.7 | 53.1 | 9.1 |
| 40.54 | 313.69 | $L_1$ | 31.4 | 3.0 | 29.3 | 32.0 |
| | | $L_2$ | 39.7 | 3.5 | 31.3 | 20.5 |
| | | $L_3$ | 50.7 | 4.4 | 26.7 | 14.5 |
| | | $L_4$ | 26.8 | 2.0 | 57.0 | 4.5 |
| 40.78 | 313.93 | $L_1$ | 33.3 | 2.5 | 30.6 | 30.3 |
| | | $L_2$ | 42.0 | 2.7 | 31.2 | 19.7 |
| | | $L_3$ | 51.5 | 3.4 | 28.3 | 13.5 |
| | | $L_4$ | 26.7 | 1.4 | 58.0 | 5.4 |
| 40.85 | 314.00 | $L_1$ | 33.5 | 2.2 | 27.4 | 33.2 |
| | | $L_2$ | 43.2 | 2.5 | 31.6 | 18.0 |
| | | $L_3$ | 53.6 | 3.0 | 25.4 | 14.4 |
| | | $L_4$ | 34.3 | 1.7 | 49.9 | 6.4 |
| 41.00 | 314.15 | $L_1$ | 29.7 | 0.2 | 24.5 | 41.5 |
| | | $L_2$ | 46.0 | 0.5 | 34.6 | 12.7 |
| | | $L_3$ | 56.2 | 0.7 | 25.8 | 12.8 |
| | | $L_4$ | 39.2 | 0.3 | 43.4 | 8.8 |
| 41.13 | 314.28 | $L_1$ | 31.5 | 2.3 | 24.2 | 37.8 |
| | | $L_2$ | 37.2 | 2.5 | 30.9 | 24.3 |
| | | $L_3$ | 46.1 | 3.2 | 26.0 | 20.4 |
| | | $L_4$ | 27.5 | 1.7 | 56.8 | 4.6 |
| 41.17 | 314.32 | $L_1$ | 29.7 | 0.2 | 24.1 | 41.7 |
| | | $L_2$ | 47.4 | 0.6 | 28.8 | 17.9 |
| | | $L_3$ | 51.8 | 0.6 | 28.1 | 14.4 |
| | | $L_4$ | 37.3 | 0.1 | 45.4 | 8.8 |
| 41.29 | 314.44 | $L_1$ | 31.7 | 0.5 | 25.1 | 39.3 |
| | | $L_2$ | 47.0 | 0.7 | 32.3 | 15.3 |
| | | $L_3$ | 53.3 | 0.8 | 27.7 | 13.8 |
| | | $L_4$ | 40.1 | 0.4 | 44.2 | 8.2 |
| 41.68 | 314.83 | $L_1$ | 36.9 | 2.7 | 25.3 | 30.6 |
| | | $L_2$ | 39.3 | 3.0 | 26.1 | 27.1 |
| | | $L_3$ | 43.8 | 3.2 | 27.7 | 20.4 |
| | | $L_4$ | 26.2 | 1.5 | 57.8 | 4.2 |

The same data are presented below in mole fractions

| $t$/°C | $T$/K (compilers) | Phase | $x_1$ (compilers) | $x_2$ (compilers) | $x_3$ (compilers) | $x_4$ (compilers) |
|---|---|---|---|---|---|---|
| 37.58 | 310.73 | $L_1$ | 0.362 | 0.040 | 0.363 | 0.110 |
| | | $L_2$ | 0.326 | 0.033 | 0.424 | 0.063 |
| | | $L_3$ | 0.602 | 0.064 | 0.219 | 0.044 |
| | | $L_4$ | 0.297 | 0.030 | 0.463 | 0.041 |
| 37.92 | 310.07 | $L_1$ | 0.364 | 0.043 | 0.359 | 0.124 |
| | | $L_2$ | 0.487 | 0.055 | 0.313 | 0.052 |
| | | $L_3$ | 0.585 | 0.062 | 0.233 | 0.044 |
| | | $L_4$ | 0.284 | 0.028 | 0.473 | 0.036 |
| 38.55 | 311.70 | $L_1$ | 0.398 | 0.037 | 0.311 | 0.125 |
| | | $L_2$ | 0.369 | 0.032 | 0.362 | 0.076 |
| | | $L_3$ | 0.640 | 0.057 | 0.187 | 0.028 |
| | | $L_4$ | 0.306 | 0.025 | 0.441 | 0.025 |
| 38.84 | 311.99 | $L_1$ | 0.346 | 0.039 | 0.333 | 0.153 |
| | | $L_2$ | 0.391 | 0.041 | 0.355 | 0.081 |
| | | $L_3$ | 0.572 | 0.056 | 0.234 | 0.046 |
| | | $L_4$ | 0.253 | 0.021 | 0.492 | 0.026 |
| 39.01 | 312.16 | $L_1$ | 0.383 | 0.027 | 0.336 | 0.108 |
| | | $L_2$ | 0.367 | 0.023 | 0.383 | 0.050 |
| | | $L_3$ | 0.627 | 0.043 | 0.204 | 0.037 |
| | | $L_4$ | 0.320 | 0.019 | 0.426 | 0.028 |
| 39.26 | 312.41 | $L_1$ | 0.362 | 0.025 | 0.348 | 0.109 |
| | | $L_2$ | 0.359 | 0.022 | 0.380 | 0.078 |
| | | $L_3$ | 0.604 | 0.039 | 0.215 | 0.044 |
| | | $L_4$ | 0.299 | 0.019 | 0.451 | 0.031 |
| 39.39 | 312.54 | $L_1$ | 0.391 | 0.040 | 0.331 | 0.131 |
| | | $L_2$ | 0.451 | 0.043 | 0.317 | 0.080 |
| | | $L_3$ | 0.570 | 0.052 | 0.244 | 0.050 |
| | | $L_4$ | 0.260 | 0.020 | 0.483 | 0.020 |
| 39.40 | 312.55 | $L_1$ | 0.404 | 0.033 | 0.340 | 0.083 |
| | | $L_2$ | 0.383 | 0.030 | 0.363 | 0.066 |
| | | $L_3$ | 0.583 | 0.047 | 0.227 | 0.048 |
| | | $L_4$ | 0.265 | 0.018 | 0.477 | 0.021 |
| 39.50 | 312.65 | $L_1$ | 0.420 | 0.033 | 0.304 | 0.114 |
| | | $L_2$ | 0.401 | 0.031 | 0.344 | 0.071 |
| | | $L_3$ | 0.603 | 0.047 | 0.216 | 0.043 |
| | | $L_4$ | 0.269 | 0.017 | 0.471 | 0.018 |
| 39.76 | 312.91 | $L_1$ | 0.339 | 0.026 | 0.312 | 0.176 |
| | | $L_2$ | 0.365 | 0.025 | 0.374 | 0.066 |
| | | $L_3$ | 0.575 | 0.038 | 0.231 | 0.050 |
| | | $L_4$ | 0.285 | 0.020 | 0.432 | 0.049 |
| 39.97 | 313.12 | $L_1$ | 0.377 | 0.023 | 0.305 | 0.154 |
| | | $L_2$ | 0.374 | 0.020 | 0.371 | 0.047 |
| | | $L_3$ | 0.614 | 0.032 | 0.212 | 0.038 |
| | | $L_4$ | 0.333 | 0.017 | 0.397 | 0.030 |
| 40.02 | 313.17 | $L_1$ | 0.342 | 0.023 | 0.393 | 0.093 |
| | | $L_2$ | 0.364 | 0.023 | 0.359 | 0.066 |
| | | $L_3$ | 0.556 | 0.035 | 0.258 | 0.044 |
| | | $L_4$ | 0.261 | 0.014 | 0.460 | 0.020 |
| 40.08 | 313.23 | $L_1$ | 0.269 | 0.016 | 0.402 | 0.196 |
| | | $L_2$ | 0.452 | 0.017 | 0.311 | 0.058 |
| | | $L_3$ | 0.528 | 0.021 | 0.272 | 0.046 |
| | | $L_4$ | 0.274 | 0.011 | 0.452 | 0.014 |
| 40.15 | 313.30 | $L_1$ | 0.384 | 0.021 | 0.320 | 0.138 |
| | | $L_2$ | 0.399 | 0.018 | 0.360 | 0.047 |
| | | $L_3$ | 0.601 | 0.030 | 0.224 | 0.039 |
| | | $L_4$ | 0.295 | 0.012 | 0.443 | 0.024 |
| 40.28 | 313.43 | $L_1$ | 0.384 | 0.022 | 0.292 | 0.153 |
| | | $L_2$ | 0.408 | 0.020 | 0.351 | 0.050 |
| | | $L_3$ | 0.601 | 0.033 | 0.221 | 0.038 |
| | | $L_4$ | 0.396 | 0.021 | 0.368 | 0.028 |
| 40.54 | 313.69 | $L_1$ | 0.358 | 0.028 | 0.329 | 0.120 |
| | | $L_2$ | 0.411 | 0.029 | 0.319 | 0.069 |
| | | $L_3$ | 0.520 | 0.037 | 0.269 | 0.049 |
| | | $L_4$ | 0.226 | 0.014 | 0.472 | 0.012 |
| 40.78 | 313.93 | $L_1$ | 0.385 | 0.023 | 0.348 | 0.115 |
| | | $L_2$ | 0.435 | 0.023 | 0.318 | 0.067 |
| | | $L_3$ | 0.525 | 0.028 | 0.284 | 0.045 |
| | | $L_4$ | 0.231 | 0.010 | 0.494 | 0.015 |
| 40.85 | 314.00 | $L_1$ | 0.391 | 0.021 | 0.315 | 0.127 |
| | | $L_2$ | 0.440 | 0.021 | 0.317 | 0.060 |
| | | $L_3$ | 0.545 | 0.025 | 0.254 | 0.048 |
| | | $L_4$ | 0.304 | 0.012 | 0.435 | 0.019 |
| 41.00 | 314.15 | $L_1$ | 0.365 | 0.002 | 0.296 | 0.167 |
| | | $L_2$ | 0.436 | 0.004 | 0.322 | 0.039 |
| | | $L_3$ | 0.553 | 0.006 | 0.250 | 0.041 |
| | | $L_4$ | 0.348 | 0.002 | 0.378 | 0.026 |
| 41.13 | 314.28 | $L_1$ | 0.376 | 0.022 | 0.284 | 0.148 |
| | | $L_2$ | 0.392 | 0.021 | 0.320 | 0.084 |
| | | $L_3$ | 0.483 | 0.027 | 0.268 | 0.070 |
| | | $L_4$ | 0.233 | 0.012 | 0.473 | 0.013 |
| 41.17 | 314.32 | $L_1$ | 0.363 | 0.002 | 0.290 | 0.167 |
| | | $L_2$ | 0.474 | 0.005 | 0.283 | 0.059 |
| | | $L_3$ | 0.510 | 0.005 | 0.272 | 0.046 |
| | | $L_4$ | 0.330 | 0.001 | 0.395 | 0.026 |
| 41.29 | 314.44 | $L_1$ | 0.390 | 0.005 | 0.304 | 0.159 |
| | | $L_2$ | 0.467 | 0.006 | 0.316 | 0.050 |
| | | $L_3$ | 0.532 | 0.006 | 0.272 | 0.045 |
| | | $L_4$ | 0.361 | 0.003 | 0.392 | 0.024 |
| 41.68 | 314.83 | $L_1$ | 0.415 | 0.025 | 0.280 | 0.113 |
| | | $L_2$ | 0.429 | 0.027 | 0.280 | 0.097 |
| | | $L_3$ | 0.452 | 0.027 | 0.281 | 0.069 |
| | | $L_4$ | 0.217 | 0.010 | 0.472 | 0.011 |

## Auxiliary Information

**Method/Apparatus/Procedure:**

The analytical method was used. The liquid mixture was placed in a glass tube 12.5 cm long with an inside diameter of 1.4 cm. The total mass of the sample was 8–10 g. The tube was closed with a Bakelite screw cap. The entire tube was mounted vertically and submerged in a water bath. After every change in temperature the sample was vigorously stirred several times using a Teflon-coated magnetic stirrer inside the tube. It was then necessary to wait from a few hours to a day for the different liquid phases to segregate into layers. Samples, typically 0.1 mL of the different phases, were removed using a syringe with a stainless steel needle. The syringe was first, if necessary, heated uniformly to a temperature (typically 50 °C) above that of the bath to prevent phase separation in the liquid. Analyses of the compositions of four coexisting phases were determined using gas chromatography.

**Source and Purity of Materials:**

(1) Fisher Chemicals; reagent grade.
(2) Aldrich Chemicals; reagent grade.
(3) Bauer Chemicals; reagent grade; contained some water.
(4) Eastman Chemicals; reagent grade.
(5) Distilled; impurity less than 0.4 mass %.

**Estimated Error:**

Temperature: ±0.01 K,
Composition: relative error less than 5%.

# 7. 1-Nitropropane: Binary and Ternary Systems

## 7.1. Water

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Water; $H_2O$; [7732-18-5]

**Evaluator:**
V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system 1-nitropropane (1)+water (2) were reported in the publications listed in Table 1.

Table 1. Summary of solubility data for the system 1-nitropropane+water

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Hankinson and Thompson[1] | 298 and 303 | mutual | synthetic |
| Pol'shinskii and Kozlov[2] | 311 | (1) in (2) | synthetic |
| Hampe[3] | 293 | mutual | not stated |
| Stephenson[4] | 273–364 | mutual | not stated |

The original data are given in the data sheets immediately following this Critical Evaluation. The data point for the nitropropane-rich phase at 303 K (Hankinson and Thompson[1]) and also in the water-rich phase at 298 K (Hankinson and Thompson[1]) is in marked disagreement with other studies and therefore rejected. All other reported data are used in Table 2 below.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in Table 2. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of 1-nitropropane (1) and water (2)

| | Water-rich phase | | | Nitropropane-rich phase | | |
|---|---|---|---|---|---|---|
| $T$/K | 100 $w_1$ | $x_1$ | | 100 $w_2$ | $x_2$ | |
| 273.2 | 1.8 | 0.0037 | tentative | 0.4 | 0.020 | tentative |
| 283.2 | 1.7 | 0.0035 | tentative | 0.5 | 0.0024 | tentative |
| 293.2 | 1.54 | 0.0032 | recommended | 0.6 | 0.0029 | tentative |
| 303.2 | 1.75 | 0.0036 | recommended | ... | ... | ... |
| 313.2 | 1.7 | 0.0035 | tentative | 1.0 | 0.048 | tentative |
| 323.2 | 1.8 | 0.0037 | tentative | 1.1 | 0.052 | tentative |
| 333.2 | 1.9 | 0.0039 | tentative | 1.4 | 0.066 | tentative |
| 343.2 | 2.0 | 0.0041 | tentative | 1.8 | 0.086 | tentative |
| 353.2 | 2.1 | 0.0043 | tentative | 1.9 | 0.087 | tentative |
| 363.2 | 2.3 | 0.0047 | tentative | 2.0 | 0.092 | tentative |

The solubility of 1-nitropropane in water ($x_1$) and solubility of water in 1-nitropropane ($x_2$) reported in the above table have been approximated by equations:

$$x_1 = 2\cdot 10^{-11}\cdot (T/\mathrm{K})^4 - 3\cdot 10^{-8}\cdot (T/\mathrm{K})^3 + 2\cdot 10^{-5}\cdot (T/\mathrm{K})^2 - 0.0044\cdot (T/\mathrm{K}) + 0.4128 \quad \text{(mean standard error of estimate was 0.0347).}$$

$$x_2 = -3\cdot 10^{-9}\cdot (T/\mathrm{K})^4 + 5\cdot 10^{-6}\cdot (T/\mathrm{K})^3 - 0.0022\cdot (T/\mathrm{K})^2 + 0.459\cdot (T/\mathrm{K}) - 36.292 \quad \text{(mean standard error of estimate was 0.0031).}$$

This relationship is presented in Fig. 12 together with experimental data reported in four studies.[1–4]

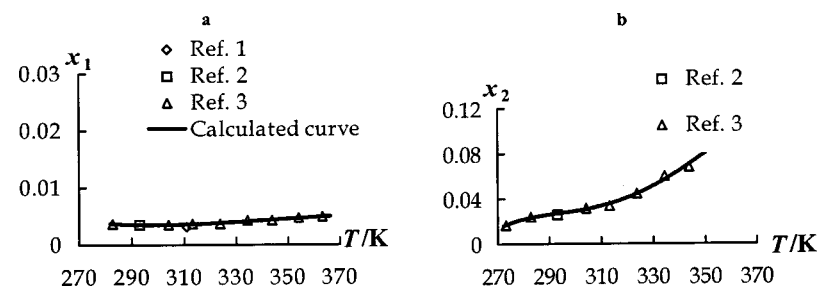


FIG. 12. Solubility of 1-nitropropane in water (a) and solubility of water in 1-nitropropane (b).

**References:**
[1]R. W. Hankinson and D. Thompson, J. Chem. Eng. Data **10**, 18 (1965).
[2]V. V. Pol'shinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9 (1970).
[3]M. J. Hampe, Chem.-Ing.-Tech. **57**, 669 (1985).
[4]R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
R. W. Hankinson and D. Thompson, J. Chem. Eng. Data **10**, 18–9 (1965).

**Variables:**
$T$/K = 298 and 303

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Mutual solubility of 1-nitropropane (1) and water (2)

| | | Water-rich phase | | 1-Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1$ | $x_1$ (compiler) | 100 $w_1$ | $x_1$ (compiler) |
| 25.00 | 298.15 | 0.9 | 0.002 | ··· | ··· |
| 30.00 | 303.15 | 1.8 | 0.004 | 99.7 | 0.985 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method of appearance and disappearance of turbidity, described in Other *et al.*[1] was used.

**Source and Purity of Materials:**
(1) Commercial Solvents Corp.; 99 mass % purity.
(2) Twice distilled.

**Estimated Error:**
Temperature: control to ±0.01 K.

**References:**
[1]D. F. Other, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
V. V. Pol'shinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9–13 (1970).

**Variables:**
$T$/K = 311

**Prepared By:**
V. P. Sazonov

**Experimental Data**
The solubility of 1-nitropropane in water at 38 °C (311 K, compiler) was reported to be 100 $w_1$ = 1.4. The corresponding mole fraction, $x_1$, calculated by the compiler is 0.0031.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method and apparatus, described in Boldarev and Kozlov[1] were used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purified; boiling point = 131.2 °C, melting point = −104.6 °C, $n$(20 °C,D) = 1.4016, $d$(20 °C,4 °C) = 1.0014.
(2) Not specified.

**Estimated Error:**
Not specified.

**References:**
[1]S. V. Boldarev and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 10 (1968).

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
M. J. Hampe, Chem.-Ing.-Tech. **57**, 669–81 (1985).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of 1-nitropropane in water at 20.0 °C (293.2 K, compiler) was reported to be 100 $w_1$ = 1.50. The corresponding mole fraction $x_1$ calculated by the compiler is 0.0031.

The solubility of water in 1-nitropropane at 20.0 °C (293.2 K, compiler) was reported to be 100 $w_2$ = 0.62. The corresponding mole fraction, $x_2$ , calculated by the compiler is 0.0299.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.

**Estimated Error:**
Not specified.

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
R. M. Stephenson, J. Chem. Eng. Data **37**, 80–95 (1992).

**Variables:**
$T$/K = 273–364

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Mutual solubility of 1-nitropropane (1) and water (2)

| | | Water-rich phase | | Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1$ | $x_1$ (compiler) | 100 $w_1$ | $x_1$ (compiler) |
| 0.0 | 273.2 | 1.78 | 0.0037 | 99.60 | 0.9805 |
| 9.5 | 282.7 | 1.65 | 0.0034 | 99.51 | 0.9762 |
| 20.0 | 293.2 | 1.58 | 0.0032 | ··· | ··· |
| 31.0 | 304.2 | 1.70 | 0.0045 | ··· | ··· |
| 41.0 | 314.2 | 1.73 | 0.0036 | 99.05 | 0.9547 |
| 50.2 | 323.4 | 1.78 | 0.0037 | 98.87 | 0.9465 |
| 60.2 | 333.4 | 1.91 | 0.0039 | 98.64 | 0.9362 |
| 70.1 | 343.3 | 2.05 | 0.0042 | 98.13 | 0.9139 |
| 81.2 | 354.4 | 2.17 | 0.0045 | 98.14 | 0.9143 |
| 90.5 | 363.7 | 2.29 | 0.0047 | 97.95 | 0.9062 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No details were reported.

**Source and Purity of Materials:**
(1) Aldrich Chemical; not purified; purity 98 mass %.
(2) Not specified.

**Estimated Error:**
Temperature: to ±0.1 K.
Composition: ±0.05 mass %.

## 7.2. Tricosane

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Tricosane; $C_{23}H_{48}$ ; [638-67-5]

**Original Measurements:**
V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (8), 9–13 (1970).

**Variables:**
$T$/K = 303–332

**Prepared by:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual solubility of 1-nitropropane and tricosane in mass percent over the specified temperature range were presented in a graphical form in the original publication. The authors at the request of the compiler provided the numerical data in the table below.

Mutual solubility of 1-nitropropane (1) and tricosane (2)

| | | Hydrocarbon-rich phase | | Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 30.0[a] | 303.2 | ··· | ··· | 99.2 | 0.998 |
| 35.0[a] | 308.2 | ··· | ··· | 97.8 | 0.994 |
| 40.0[a] | 313.2 | ··· | ··· | 94.2 | 0.983 |
| 45.3[a] | 318.5 | 22.0 | 0.507 | 89.7 | 0.969 |
| 46.0[a] | 319.2 | 11.2 | 0.315 | ··· | ··· |
| 48.8[b] | 322.0 | 31.7 | 0.628 | ··· | ··· |
| 51.8[b] | 325.0 | 39.7 | 0.706 | ··· | ··· |
| 52.1[b] | 325.3 | ··· | ··· | 83.3 | 0.948 |
| 54.5[b] | 327.7 | 45.0 | 0.749 | ··· | ··· |
| 54.6[b] | 327.8 | ··· | ··· | 80.0 | 0.936 |
| 55.6[b] | 328.8 | 47.7 | 0.769 | ··· | ··· |
| 56.9[b] | 329.1 | ··· | ··· | 74.7 | 0.915 |
| 57.7[b] | 330.0 | 55.8 | 0.821 | ··· | ··· |
| 58.5[b] | 331.7 | 65.0 | 0.871 | 65.0 | 0.871 (UCST) |

[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium occurs at 45.3 °C (318.5 K, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; boiling point = 383.8 °C, melting point = 47.7 °C.

**Estimated Error:**
Not reported.

## 7.3. Oils

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Oils

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (4), 26–8 (1968).

**Variables:**
$T$/K = 275–336

**Prepared By:**
V. P. Sazonov

**Experimental Data**

Solubility temperatures of 1-nitropropane (1) and oil (2) mixtures ratio 3:1

| Oil | Freezing Point oil/°C | Kinematic viscosity oil/cS | $t$/°C | $T$/K (compiler) |
|---|---|---|---|---|
| Diesel fuel | −56 | 8.05 (20 °C) | 1.5 | 274.7 |
| Distillate oil | −45.5 | 7.84 (50 °C) | 30.5 | 303.7 |
| Distillate oil | −33 | 16.05 (50 °C) | 35.5 | 308.7 |
| Distillate oil | −27 | 6.28 (100 °C) | 55.2 | 328.4 |
| Residual oil | −18 | 20.55 (100 °C) | 63.2 | 336.4 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No details were reported.

**Source and Purity of Materials:**
(1) Not specified.
(2) Prepared from Tuimazin crude oil.

**Estimated Error:**
Not specified.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 7.4. Paraffins

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Paraffins;

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (8), 26–8 (1968).

**Variables:**
$T$/K= 255–313

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

### Experimental Data

The solubilities of paraffins in 1-nitropropane over the indicated temperature range were presented in graphically as a plot of temperature against log solubility. The data in the table below were extracted compilers from the reported graphs.

Solubility of paraffins (2) in 1-nitropropane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| | | Paraffin* | | |
| −18.1 | 255.1 | 0.1 | 0.1 | 0.0004 |
| −13.6 | 259.6 | 0.3 | 0.3 | 0.0012 |
| −10.0 | 263.2 | 0.5 | 0.5 | 0.0020 |
| −8.3 | 264.9 | 0.7 | 0.7 | 0.0029 |
| −3.6 | 269.6 | 1.0 | 1.0 | 0.0041 |
| 6.1 | 279.3 | 3.0 | 2.9 | 0.0121 |
| 10.0 | 283.2 | 5.0 | 4.8 | 0.0202 |
| 12.6 | 285.8 | 7.0 | 6.5 | 0.0276 |
| | | Paraffin** | | |
| −1.6 | 271.6 | 0.1 | 0.1 | 0.0004 |
| 5.2 | 278.4 | 0.3 | 0.3 | 0.0011 |
| 8.9 | 282.1 | 0.5 | 0.5 | 0.0018 |
| 13.1 | 286.3 | 0.7 | 0.7 | 0.0025 |
| 15.8 | 289.0 | 1.0 | 1.0 | 0.0035 |
| 25.6 | 298.8 | 3.9 | 3.8 | 0.0136 |
| 27.1 | 300.3 | 5.0 | 4.8 | 0.0173 |
| | | Paraffin*** | | |
| 4.8 | 278.0 | 0.055 | 0.055 | 0.0002 |
| 7.8 | 281.0 | 0.07 | 0.07 | 0.0002 |
| 11.6 | 284.8 | 0.11 | 0.11 | 0.0003 |
| 20.0 | 293.2 | 0.3 | 0.3 | 0.0009 |
| 26.3 | 299.5 | 0.7 | 0.7 | 0.0021 |
| 28.8 | 302.0 | 1.3 | 1.3 | 0.0039 |
| | | Paraffin**** | | |
| 2.3 | 275.5 | 0.01 | 0.01 | 0.00003 |
| 15.3 | 288.5 | 0.05 | 0.05 | 0.0001 |
| 20.0 | 293.2 | 0.08 | 0.08 | 0.0002 |
| 23.8 | 297.0 | 0.1 | 0.1 | 0.0003 |
| 32.0 | 305.2 | 0.3 | 0.3 | 0.0008 |
| 34.3 | 307.5 | 0.5 | 0.5 | 0.0013 |
| 38.0 | 311.2 | 0.7 | 0.7 | 0.0019 |
| 40.0 | 313.2 | 1.0 | 1.0 | 0.0027 |

NOTE: Footnotes explained in Source and Purity of Materials section, below.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Obtained by separation of narrow fraction with boiling point*=196–270 °C, boiling point**=300–365 °C from a wide fraction of diesel fuel; melting point*=13.2 °C and melting point**=28.0 °C; *** and **** obtained by separation of the third oil fraction of Tuimazin crude; melting point***=41.7 °C and melting point****=50.7 °C.

**Estimated Error:**
Not reported.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 7.5. Uranium bis (nitrato-O) Dioxohexahydrate

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Uranium bis (nitrato-O) dioxohexahydrate; $UO_2(NO_3)_2 \cdot 6H_2O$; [13520-83-7]

**Original Measurements:**
R. K. Warner, Austral. J. Appl. Sci. **4**, 581–9 (1953).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of uranyl nitrate (2) in 1-nitropropane (1) at 20 °C (293 K, compiler) was reported to be 100 $w_2$ = 1.1. The corresponding mole fraction, $x_2$ , calculated by the compiler, is 0.003.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The analytical method was used. A sample of (2) was placed with the appropriate amount of pure (1) in a small flask. The contents of the flask were warmed to 30–50 °C, agitated with excess crystals of (2) for 15 min, and then placed in a constant temperature bath at 20 °C with intermittent shaking for 6–8 h. Crystallization from the supersaturated solution occurred, and when equilibrium was reached the solution was quickly decanted, filtered to remore fine crystals, and placed in a stoppered flask at 20 °C for analysis.

**Source and Purity of Materials:**
(1) Synthesized by standard method; thoroughly dried and fractionally distilled.
(2) Source not specified; A.R. grade; not purified.

**Estimated Error:**
Temperature: ±0.05 K, solubility: ±0.2 g/100 g solution.

## 7.6. Methanol+Water

**Components:**
(1) 1-Nitropropane; $C_3H_7NO_2$ ; [108-03-2]
(2) Methanol; $CH_4O$; [67-56-1]
(3) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
R. W. Hankinson and D. Thompson, J. Chem. Eng. Data **10**, 18–9 (1965).

**Variables:**
$T$/K = 298 and 303

**Prepared By:**
V. P. Sazonov and M. F. Chernysheva

**Experimental Data**

Table 1. Mutual solubility of 1-nitropropane (1), methanol (2), and water (3)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | 100 $w_2$ | $x_1$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|---|
| 25.00 | 298.15 | 2.1 | 13.3 | 0.005 | 0.081 |
| | | 2.7 | 23.3 | 0.006 | 0.150 |
| | | 3.1 | 31.1 | 0.007 | 0.209 |
| | | 5.2 | 36.7 | 0.013 | 0.259 |
| | | 7.3 | 40.9 | 0.019 | 0.302 |
| | | 9.2 | 44.1 | 0.025 | 0.339 |
| | | 12.0 | 46.1 | 0.035 | 0.370 |
| | | 13.8 | 48.1 | 0.041 | 0.399 |
| | | 28.8 | 45.7 | 0.102 | 0.452 |
| | | 34.2 | 43.5 | 0.129 | 0.457 |
| | | 41.8 | 39.9 | 0.173 | 0.458 |
| | | 52.9 | 33.6 | 0.249 | 0.439 |
| | | 61.6 | 27.9 | 0.323 | 0.407 |
| | | 71.7 | 22.7 | 0.443 | 0.390 |
| | | 83.4 | 13.2 | 0.611 | 0.269 |
| 30.00 | 303.15 | 2.4 | 13.3 | 0.005 | 0.081 |
| | | 3.2 | 23.2 | 0.007 | 0.150 |
| | | 4.1 | 27.2 | 0.010 | 0.181 |
| | | 4.5 | 30.7 | 0.011 | 0.208 |
| | | 6.4 | 36.3 | 0.016 | 0.259 |
| | | 8.6 | 40.3 | 0.023 | 0.301 |
| | | 10.8 | 43.4 | 0.030 | 0.338 |
| | | 13.8 | 45.4 | 0.040 | 0.369 |
| | | 16.0 | 45.6 | 0.048 | 0.382 |
| | | 19.1 | 46.4 | 0.060 | 0.405 |
| | | 22.8 | 46.3 | 0.075 | 0.424 |
| | | 27.3 | 45.3 | 0.095 | 0.438 |
| | | 21.7 | 51.8 | 0.073 | 0.486 |
| | | 28.3 | 45.1 | 0.100 | 0.441 |
| | | 41.0 | 39.2 | 0.166 | 0.441 |
| | | 52.3 | 33.3 | 0.243 | 0.430 |
| | | 61.3 | 27.9 | 0.320 | 0.404 |
| | | 70.0 | 22.3 | 0.414 | 0.367 |
| | | 82.9 | 13.2 | 0.599 | 0.265 |

Table 2. Composition of two liquid phases at equilibrium

| $t$/°C | $T$/K (compilers) | 1-Nitropropane-rich phase | | Water-rich phase | | 1-Nitropropane-rich phase (compilers) | | Water-rich phase (compilers) | |
|---|---|---|---|---|---|---|---|---|---|
| | | $100\ w_1'$ | $100\ w_2'$ | $100\ w_1''$ | $100\ w_2''$ | $x_1'$ | $x_2'$ | $x_1''$ | $x_2''$ |
| 25.00 | 298.15 | 93.9 | 4.7 | 3.0 | 19.9 | 0.824 | 0.115 | 0.007 | 0.126 |
| | | 86.9 | 10.2 | 3.2 | 22.9 | 0.671 | 0.219 | 0.007 | 0.147 |
| | | 75.2 | 19.5 | 3.6 | 28.4 | 0.484 | 0.348 | 0.008 | 0.189 |
| | | 65.2 | 26.1 | 4.5 | 32.3 | 0.361 | 0.401 | 0.011 | 0.221 |
| | | 54.2 | 32.9 | 6.1 | 37.9 | 0.259 | 0.437 | 0.016 | 0.271 |
| | | 48.1 | 35.9 | 8.4 | 42.3 | 0.211 | 0.439 | 0.023 | 0.318 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Two methods were used. The solubility data were determined by a modification of the "cloud point" method described in Other *et al.*[1] 20 mL mixtures of (2) and (3) were placed in flasks, sealed and immersed in a constant temperature bath for approximately 4 h. Each container in turn was opened, and the contents titrated from calibrated burettes of (1). The (1)-rich portion of the solubility curve was obtained by reversing the procedure. The vessel containing the titrated mixture was continually agitated in a constant temperature bath. The equilibrium data were determined by the synthetic method described in Other *et al.*[1] Solutions consisting of all three components were made. These two-phase mixtures were then sealed in polyethylene containers and placed in the constant temperature bath. Each container was removed from the constant temperature bath, then the two phases were separated, and the refractive index of each phase was determined.

**Source and Purity of Materials:**

(1) Commercial Solvents Corp.; 99 mass % purity.
(2) Source not specified; purity not specified; distilled with a boiling range of ±0.1 K.
(3) Twice distilled.

**Estimated Error:**

Temperature: control: ±0.01 K.

**References:**

[1]D. F. Other, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

# 8. 2-Nitropropane: Binary Systems

## 8.1. Water

**Components:**

(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Water; $H_2O$; [7732-18-5]

**Evaluator:**

V. P. Sazonov, Technical University, Samara, Russia, May, 2000.

**Critical Evaluation**

Quantitative solubility data for the system 2-nitropropane (1)+water (2) were reported in the publications listed in Table 1.

Table 1. Summary of solubility data for the system 2-nitropropane+water

| Reference | $T$/K | Solubility | Method |
|---|---|---|---|
| Pol'shinskii and Kozlov[1] | 311 | (1) in (2) | synthetic |
| Hampe[2] | 293 | mutual | not stated |
| Stephenson[3] | 273–364 | mutual | not stated |

The original data are given in the data sheets immediately following this Critical Evaluation. All reported data are used in the table below.

Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are presented in the Table 2. Data are "recommended" if two or more apparently reliable studies are in reasonable (±5% relative) agreement. All other data are regarded as tentative only.

Table 2. Recommended and tentative values for the mutual solubilities of 2-nitropropane (1) and water (2)

| $T$/K | water-rich phase | | | 2-nitropropane-rich phase | | |
|---|---|---|---|---|---|---|
| | $100\ w_1$ | $x_1$ | | $100\ w_2$ | $x_2$ | |
| 273.2 | 3.0 | 0.0062 | tentative | 0.3 | 0.015 | tentative |
| 293.2 | 1.75 | 0.0036 | recommended | 0.5 | 0.024 | recommended |
| 303.2 | 1.7 | 0.0035 | tentative | 0.6 | 0.029 | tentative |
| 313.2 | 1.75 | 0.0036 | recommended | 0.7 | 0.034 | tentative |
| 323.2 | 1.8 | 0.0037 | tentative | 1.0 | 0.048 | tentative |
| 333.2 | 2.0 | 0.0041 | tentative | 1.2 | 0.057 | tentative |
| 343.2 | 2.0 | 0.0041 | tentative | 1.4 | 0.066 | tentative |
| 353.2 | 2.2 | 0.0045 | tentative | 1.9 | 0.087 | tentative |
| 363.2 | 2.4 | 0.0049 | tentative | 2.3 | 0.104 | tentative |

The solubility of 2-nitropropane in water ($x_1$) and solubility of water in 2-nitropropane ($x_2$) reported in the above table have been approximated by equations:

$$x_1 = 3\cdot 10^{-13}\cdot (T/\mathrm{K})^6 - 5\cdot 10^{-10}\cdot (T/\mathrm{K})^5 + 4\cdot 10^{-7}\cdot (T/\mathrm{K})^4 - 2\cdot 10^{-4}\cdot (T/\mathrm{K})^3 + 0.0452\cdot (T/\mathrm{K})^2 - 5.8977\cdot (T/\mathrm{K}) + 319.61,$$

$$x_2 = -4\cdot 10^{-9}\cdot (T/\mathrm{K})^4 + 5\cdot 10^{-6}\cdot (T/\mathrm{K})^3 - 0.0021\cdot (T/\mathrm{K})^2 + 0.4279\cdot (T/\mathrm{K}) - 32.508,$$

(mean standard error of estimate was 0.0112).

This relationship is presented in Fig. 13 together with experimental data as reported in three studies.[1–3]

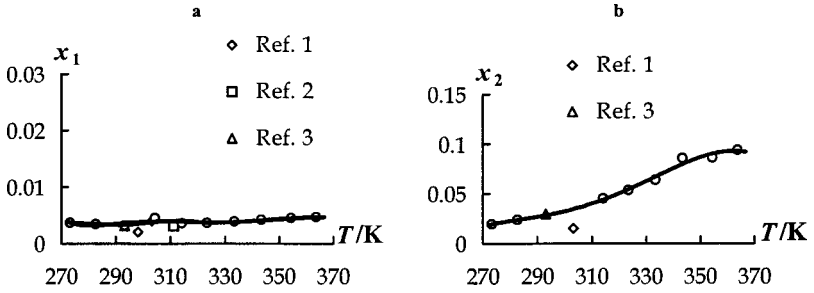


FIG. 13. Solubility of 2-nitropropane in water (a) and solubility of water in 2-nitropropane (b).

**References:**

[1]V. V. Pol'shinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9 (1970).

[2]M. J. Hampe, Chem.-Ing.-Tech. **57**, 669 (1985).

[3]R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
V. V. Pol'shinskii and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 9–13 (1970).

**Variables:**
$T$/K = 311

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of 2-nitropropane in water at 38 °C (311 K, compiler) was reported to be $100\,w_1 = 1.7$. The corresponding mole fraction $x_1$ calculated by the compiler is 0.0031.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method and apparatus, described in Boldarev and Kozlov[1] were used. No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purified; boiling point = 120.3 °C, melting point = −91.3 °C, $n$(20 °C,D) = 1.3944, $d$(20 °C,4 °C) = 0.9884.
(2) Not specified.

**Estimated Error:**
Not specified.

**References:**
[1]S. V. Boldarev and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (10), 10 (1968).

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
M. J. Hampe, Chem.-Ing.-Tech. **57**, 669–81 (1985).

**Variables:**
$T$/K = 293

**Prepared By:**
V. P. Sazonov

**Experimental Data**

The solubility of 2-nitropropane in water at 20 °C (293 K, compiler) was reported to be 100 $w_1$ = 1.71. The corresponding mole fraction $x_1$ calculated by the compiler is 0.0035.

The solubility of water in 1-nitropropane at 20 °C (293 K, compiler) was reported to be 100 $w_2$ = 0.53. The corresponding mole fraction $x_2$ calculated by the compiler is 0.0257.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Not specified.

**Estimated Error:**
Not specified.

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Water; $H_2O$; [7732-18-5]

**Original Measurements:**
R. M. Stephenson, J. Chem. Eng. Data **37**, 80–95 (1992).

**Variables:**
$T$/K = 273–363

**Prepared By:**
V. P. Sazonov

**Experimental Data**

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

| | | Water-rich phase | | 2-Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | 100 $w_1$ | $x_1$ (compiler) | 100 $w_1$ | $x_1$ (compiler) |
| 0.0 | 273.2 | 3.07 | 0.0064 | 99.66 | 0.9834 |
| 19.7 | 282.9 | 1.80 | 0.0037 | 99.51 | 0.9762 |
| 30.9 | 304.1 | 1.70 | 0.0035 | 99.35 | 0.9687 |
| 40.0 | 313.2 | 1.78 | 0.0037 | 99.30 | 0.9663 |
| 50.5 | 323.7 | 1.79 | 0.0037 | 99.07 | 0.9556 |
| 61.1 | 334.3 | 2.07 | 0.0043 | 98.73 | 0.9402 |
| 70.6 | 343.8 | 2.09 | 0.0043 | 98.55 | 0.9322 |
| 81.0 | 354.2 | 2.26 | 0.0047 | 98.09 | 0.9122 |
| 90.2 | 363.4 | 2.36 | 0.0049 | 97.77 | 0.8987 |

Below 10 °C, organic-rich phase on bottom; above 10 °C, organic-rich phase top.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
No details were reported.

**Source and Purity of Materials:**
(1) Aldrich Chemical; not purified; purity 96 mass %.
(2) Not specified.

**Estimated Error:**
Temperature: to 0.1 K,
Composition: 0.03 mass %.

## 8.2. Benezene

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Benzene; $C_6H_6$ ; [71-43-2]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and M. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 177–279

**Prepared By:**
V. P. Sazonov

**Experimental Data**
No region of liquid–liquid immiscibility was observed. A full solid–liquid phase diagram is presented.

Solubility of 2-nitropropane (1) and benzene (2)

| $t$/°C | $T$/K (compiler) | $x_1$ | 100 $w_1$ (compiler) |
|---|---|---|---|
| −96.11 | 177.04 | 0.924 | 93.3 |
| −94.97 | 178.18 | 0.962 | 96.7 |
| −91.50 | 181.65 | 1.000 | 100.0 |
| −76.52 | 196.63 | 0.845 | 86.1 |
| −39.66 | 233.49 | 0.581 | 61.3 |
| −30.13 | 243.02 | 0.497 | 53.0 |
| −14.84 | 258.31 | 0.335 | 36.5 |
| −9.89 | 263.26 | 0.249 | 27.4 |
| −5.72 | 267.43 | 0.165 | 18.4 |
| −3.92 | 269.23 | 0.129 | 14.5 |
| −0.80 | 272.35 | 0.09 | 10.1 |
| 0.31 | 273.46 | 0.0721 | 8.14 |
| 2.00 | 275.15 | 0.0553 | 6.26 |
| 3.06 | 276.21 | 0.0374 | 4.24 |
| 5.45 | 278.60 | 0.0 | 0.0 |

A eutectic was reported at (−98 °C) at $x_1$ = 0.93 (100 $w_1$ = 93.8, compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Cooling curves were run on a Precision Scientific Co. freezing point apparatus equipped with a Leeds and Northrup Co. Mueller bridge and platinum resistance thermometer. The minimum sample size was 50 mL. Usually a (1) and (2) solution was prepared, a cooling curve taken, a known amount of (1) added, and a second cooling curve taken. The procedure was then repeated with a new sample. Only ordinary precautions were taken to exclude water from the system. Either dry ice–acetone or liquid nitrogen was used as the coolant around the evacuated Dewar flask holding the sample.

**Source and Purity of Materials:**
(1) Eastman; practical grade; distilled at 60 °C/13.3 kPa.
(2) Fisher ACS certified.

**Estimated Error:**
Not specified.

## 8.3. Nonane

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Nonane; $C_9H_{20}$ ; [111-84-2]

**Original Measurements:**
H. L. Clever, Q. R. Pirkle, Jr., B. J. Allen, Jr., and N. E. Derrick, J. Chem. Eng. Data **17**, 31–4 (1972).

**Variables:**
$T$/K = 254–269

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Mutual solubility of 2-nitropropane (1) and nonane (2)

| | | Nonane-rich phase | | 2-Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compiler) | $x_1$ | 100 $w_1$ (compiler) | $x_1$ | 100 $w_1$ (compiler) |
| −19.1 | 254.1 | ··· | ··· | 0.865 | 81.7 |
| −7.8 | 265.4 | ··· | ··· | 0.775 | 70.5 |
| −5.3 | 267.9 | ··· | ··· | 0.680 | 59.6 |
| −4.8 | 268.4 | 0.425 | 33.9 | ··· | ··· |
| −4.6 | 268.6 | ··· | ··· | 0.550 | 45.9 |
| −4.5 | 268.7 | ··· | ··· | ··· | ··· (UCST) |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. The solutions of (1) and (2) were sealed in 5 mL glass vials. The cloud points were observed visually in an acetone bath slowly cooled by the addition of portions of dry ice. Temperatures were observed on an alcohol thermometer.

**Source and Purity of Materials:**
(1) Eastman; practical grade; distilled at 60 °C/13.3 kPa.
(2) Phillips; purity 99 mol %.

**Estimated Error:**
Not specified.

## 8.4. Tricosane

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Tricosane; $C_{23}H_{48}$ ; [638-67-5]

**Original Measurements:**
V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (8), 9–13 (1970).

**Variables:**
$T$/K = 303–325

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

The mutual solubility of 2-nitropropane (1) and tricosane (2) in mass percent over the specified temperature range were presented in a graphical form in the original publication. The authors at the request of the compilers provided the numerical data in the table below.

Mutual solubility of 2-nitropropane (1) and tricosane (2)

| | | Hydrocarbon-rich phase | | 2-Nitropropane-rich phase | |
|---|---|---|---|---|---|
| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) | 100 $w_1$ | $x_1$ (compilers) |
| 30.0[a] | 303.2 | ··· | ··· | 97.8 | 0.994 |
| 35.0[a] | 308.2 | ··· | ··· | 96.2 | 0.989 |
| 40.0[a] | 313.2 | ··· | ··· | 92.2 | 0.977 |
| 43.3[a] | 316.5 | 33.8 | 0.650 | 88.0 | 0.964 |
| 44.6[a] | 317.8 | 17.0 | 0.427 | ··· | ··· |
| 46.9[a] | 320.1 | 2.5 | 0.085 | ··· | ··· |
| 47.5[b] | 320.7 | ··· | ··· | 81.2 | 0.940 |
| 47.9[b] | 321.1 | 45.3 | 0.751 | ··· | ··· |
| 50.0[b] | 323.2 | ··· | ··· | 75.0 | 0.916 |
| 50.8[b] | 324.0 | 54.5 | 0.814 | ··· | ··· |
| 51.8[b] | 325.0 | 64.2 | 0.867 | 64.2 | 0.867 (UCST) |

[a]Solid–liquid equilibrium.
[b]Liquid–liquid equilibrium.

Monotectic equilibrium occurs at 43.3 °C (316.5 K, compilers).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; boiling point = 383.8 °C, melting point = 47.7 °C.

**Estimated Error:**
Not reported.

## 8.5. Oils

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Oils

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (4), 26–8 (1968).

**Variables:**
$T$/K = 274–336

**Prepared By:**
V. P. Sazonov

**Experimental Data**

Solubility temperatures of 2-nitropropane (1) and oil (2) mixtures ratio 3:1

| Oil | Freezing point oil/°C | Kinematic viscosity oil/cS | $t$/°C | $T$/K (compiler) |
|---|---|---|---|---|
| Diesel fuel | −56 | 8.05 (20 °C) | 0.5 | 273.7 |
| Distillate oil | −45.5 | 7.84 (50 °C) | 29.5 | 302.7 |
| Distillate oil | −33 | 16.05 (50 °C) | 35.0 | 308.2 |
| Distillate oil | −27 | 6.28 (100 °C) | 43.5 | 316.7 |
| Residual oil | −18 | 20.55 (100 °C) | 62.5 | 335.7 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Prepared from Tuimazin crude oil.

**Estimated Error:**
Not specified.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 8.6. Paraffins

**Components:**
(1) 2-Nitropropane; $C_3H_7NO_2$ ; [79-46-9]
(2) Paraffins

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (8), 26–8 (1968).

**Variables:**
$T$/K= 250–312

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

### Experimental Data

The solubilities of paraffins in 2-nitropropane over the indicated temperature range were presented graphically as plots of temperature against log solubility. The data in the table below were extracted compiler from the reported graphs.

Solubility of paraffins (2) in 2-nitropropane (1)

| $t$/°C | $T$/K (compiler) | $g_2$/100 $g_1$ | 100 $w_2$ (compiler) | $x_2$ (compiler) |
|---|---|---|---|---|
| | | Paraffin* | | |
| −23.6 | 249.6 | 0.1 | 0.1 | 0.0004 |
| −18.7 | 254.5 | 0.3 | 0.3 | 0.0012 |
| −11.4 | 261.8 | 0.5 | 0.5 | 0.0020 |
| −8.6 | 264.6 | 0.7 | 0.7 | 0.0029 |
| −5.0 | 268.2 | 1.0 | 1.0 | 0.0041 |
| 5.0 | 278.2 | 3.0 | 2.9 | 0.0121 |
| 8.6 | 281.8 | 5.0 | 4.8 | 0.0202 |
| 11.4 | 284.6 | 7.0 | 6.5 | 0.0276 |
| | | Paraffin** | | |
| −7.2 | 266.0 | 0.07 | 0.07 | 0.0003 |
| −2.8 | 270.4 | 0.1 | 0.1 | 0.0004 |
| 4.1 | 277.3 | 0.3 | 0.3 | 0.0011 |
| 8.0 | 281.2 | 0.5 | 0.5 | 0.0018 |
| 10.9 | 284.1 | 0.7 | 0.7 | 0.0025 |
| 14.8 | 288.0 | 1.0 | 1.0 | 0.0035 |
| 24.3 | 297.5 | 3.9 | 3.8 | 0.0136 |
| 26.3 | 299.5 | 5.0 | 4.8 | 0.0173 |
| | | Paraffin*** | | |
| 3.8 | 277.0 | 0.055 | 0.055 | 0.0002 |
| 10.0 | 283.2 | 0.07 | 0.07 | 0.0002 |
| 18.2 | 291.4 | 0.11 | 0.11 | 0.0003 |
| 22.5 | 295.7 | 0.3 | 0.3 | 0.0009 |
| 25.0 | 298.2 | 0.7 | 0.7 | 0.0021 |
| 27.9 | 301.1 | 1.3 | 1.3 | 0.0039 |
| | | Paraffin**** | | |
| 1.3 | 274.5 | 0.01 | 0.01 | 0.00003 |
| 14.3 | 287.5 | 0.05 | 0.05 | 0.0001 |
| 20.0 | 293.2 | 0.08 | 0.08 | 0.0002 |
| 21.9 | 295.1 | 0.1 | 0.1 | 0.0003 |
| 30.3 | 303.5 | 0.3 | 0.3 | 0.0008 |
| 32.9 | 306.1 | 0.5 | 0.5 | 0.0013 |
| 35.8 | 309.0 | 0.7 | 0.7 | 0.0019 |
| 38.8 | 312.0 | 1.0 | 1.0 | 0.0027 |

NOTE: Footnotes explained in Source and Purity of Materials section, below.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Obtained by separation of narrow fraction with boiling point*=196–270 °C and boiling point**=300–365 °C from a wide fraction of diesel fuel; melting point*=13.2 °C and melting point**=28.0 °C; *** and **** obtained by separation of the third oil fraction of Tuimazin crude; melting point***=41.7 °C and melting point****=50.7 °C.

**Estimated Error:**
Not reported.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

# 9. 2-Nitrobutane: Binary Systems

## 9.1 Tricosane

**Components:**
(1) 2-Nitrobutane; $C_4H_9NO_2$ ; [600-24-8]
(2) Tricosane; $C_{23}H_{48}$ ; [638-67-5]

**Original Measurements:**
V. A. Rakhmanova and L. M. Kozlov, Khim. Tekhnol. Topl. Masel (8), 9–13 (1970).

**Variables:**
$T$/K = 298–319

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

**Experimental Data**

No region of liquid–liquid immiscibility was observed. The solubility of 2-nitrobutane (1) and tricosane (2) in mass percent over the specified temperature range were presented in a graphical form in the original publication. The authors at the request of the compilers provided the numerical data in the table below.

Solubility of 2-nitrobutane (1) and tricosane (2)

| $t$/°C | $T$/K (compilers) | 100 $w_1$ | $x_1$ (compilers) |
|---|---|---|---|
| 25.0 | 298.2 | 98.3 | 0.995 |
| 30.0 | 303.2 | 96.5 | 0.989 |
| 35.0 | 308.2 | 92.5 | 0.975 |
| 38.7 | 311.9 | 85.0 | 0.947 |
| 40.5 | 313.7 | 73.7 | 0.898 |
| 40.8 | 314.0 | 64.5 | 0.851 |
| 41.1 | 314.3 | 53.3 | 0.782 |
| 41.3 | 314.5 | 41.7 | 0.693 |
| 41.7 | 314.9 | 31.7 | 0.594 |
| 42.5 | 315.7 | 23.0 | 0.485 |
| 44.0 | 317.2 | 13.7 | 0.333 |
| 46.0 | 319.2 | 5.8 | 0.162 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The synthetic method was used. No details were reported.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified.
(2) Source not specified; purity not specified; boiling point = 383.8 °C, melting point = 47.7 °C.

**Estimated Error:**
Not reported.

## 9.2. Oils

**Components:**
(1) 2-Nitrobutane; $C_4H_9NO_2$ ; [600-24-8]
(2) Oils

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (4), 26–8 (1968).

**Variables:**
$T$/K = 243–299

**Prepared By:**
V. P. Sazonov

**Experimental Data**

Solubility temperatures of 2-nitrobutane (1) and oil (2) mixtures ratio 3:1

| Oil | Freezing point oil/°C | Kinematic viscosity oil/cS | $t$/°C | $T$/K (compiler) |
|---|---|---|---|---|
| Diesel fuel | −56 | 8.05 (20 °C) | −30 | 243.2 |
| Distillate oil | −45.5 | 7.84 (50 °C) | −6 | 267.2 |
| Distillate oil | −33 | 16.05 (50 °C) | −1 | 272.2 |
| Distillate oil | −27 | 6.28 (100 °C) | 7.5 | 280.7 |
| Residual oil | −18 | 20.55 (100 °C) | 25.5 | 298.7 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Prepared from Tuimazin crude oil.

**Estimated Error:**
Not specified.

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 9.3. Paraffins

**Components:**
(1) 2-Nitrobutane; $C_4H_9NO_2$ ; [600-24-8]
(2) Paraffins

**Original Measurements:**
L. M. Kozlov and V. I. Volpert, Khim. Tekhnol. Topl. Masel (8), 26–8 (1968).

**Variables:**
$T$/K= 255–307

**Prepared By:**
V. P. Sazonov and N. V. Sazonov

### Experimental Data

The solubilities of paraffins (2) in 2-nitrobutane (1) over the indicated temperature range were presented graphically as a plots of temperature against log solubility. The data in the table below were extracted compiler from the reported graphs.

Solubility of paraffins (2) in 2-nitrobutane (1)

| $t$/°C | $T$/K (compilers) | $g_2$/100 $g_1$ | 100 $w_2$ (compilers) | $x_2$ (compilers) |
|---|---|---|---|---|
| | | Paraffin* | | |
| −17.9 | 255.3 | 0.5 | 0.5 | 0.0024 |
| −15.7 | 257.5 | 0.7 | 0.7 | 0.0033 |
| −12.1 | 261.1 | 1.1 | 1.1 | 0.0052 |
| −2.9 | 270.3 | 3.0 | 2.9 | 0.0139 |
| 2.1 | 275.3 | 5.0 | 4.8 | 0.0233 |
| | | Paraffin** | | |
| −10.0 | 263.2 | 0.1 | 0.1 | 0.0004 |
| −2.2 | 271.0 | 0.3 | 0.3 | 0.0012 |
| 2.2 | 275.4 | 0.5 | 0.5 | 0.0020 |
| 4.2 | 277.4 | 0.7 | 0.7 | 0.0028 |
| 6.1 | 279.3 | 1.0 | 1.0 | 0.0041 |
| 8.0 | 281.2 | 4.0 | 3.8 | 0.0158 |
| | | Paraffin*** | | |
| 4.1 | 277.3 | 0.1 | 0.1 | 0.0003 |
| 12.9 | 286.1 | 0.3 | 0.3 | 0.0010 |
| 16.6 | 289.8 | 0.6 | 0.6 | 0.0021 |
| 18.6 | 291.8 | 0.7 | 0.7 | 0.0024 |
| 20.5 | 293.7 | 1.2 | 1.2 | 0.0041 |
| 26.3 | 299.5 | 2.7 | 2.6 | 0.0091 |
| | | Paraffin**** | | |
| 10.0 | 283.2 | 0.05 | 0.05 | 0.0002 |
| 13.8 | 287.0 | 0.08 | 0.08 | 0.0002 |
| 16.5 | 289.7 | 0.1 | 0.1 | 0.0003 |
| 25.0 | 298.2 | 0.3 | 0.3 | 0.0009 |
| 29.0 | 302.2 | 0.5 | 0.5 | 0.0015 |
| 31.0 | 304.2 | 0.7 | 0.7 | 0.0021 |
| 33.8 | 307.0 | 1.0 | 1.0 | 0.0031 |

NOTE: Footnotes explained in Source and Purity of Materials section, below.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The method, described in Poole[1] was used. No experimental details given.

**Source and Purity of Materials:**
(1) Not specified.
(2) Obtained by separation of narrow fraction with boiling point*=196–270 °C and boiling point**=300–365 °C from a wide fraction of diesel fuel; melting point*=13.2 °C and melting point**=28.0 °C; *** and **** obtained by separation of the third oil fraction of Tuimazin crude; melting point***=41.7 °C and melting point****=50.7 °C.

**Estimated Error:**
Not reported

**References:**
[1]G. W. Poole, Ind. Eng. Chem. **21**, 1098 (1929).

## 9.4. Nitrobutane+Trichlorofluoromethane

**Components:**
(1) Nitrobutane; $C_4H_9NO_2$; [627-05-4]
(2) Trichlorofluoromethane; $CCl_3F$; [75-69-4]

**Original Measurements:**
M. J. Copley, G. F. Zellhoefer, and C. S. Marvel, J. Am. Chem. Soc. **61**, 3550–2 (1939).

**Variables:**
$T$/K=305

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Solubility of trichlorofluoromethane (2) in nitrobutane (1)

| $t$/°C | $T$/K (compiler) | $g_2/100\,g_1$ | $100\,w_2$ (compiler) | $x_2$ (compiler) |
|---|---|---|---|---|
| 32.2 | 305.4 | 35.6 | 26.3 | 0.210 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The procedure followed in making the solubility measurements described in Zellhoefer.[1] No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified by distillation.
(2) Source not specified; purity not specified.

**Estimated Error:**
Solubility: reproducible to within 1%.

**References:**
[1]G. F. Zellhoefer, Ind. Eng. Chem. **37**, 584 (1939).

## 9.5. Nitrobutane+Dichlorofluoromethane

**Components:**
(1) Nitrobutane; $C_4H_9NO_2$; [627-05-4]
(2) Dichlorofluoromethane; $CHCl_2F$; [75-43-4]

**Original Measurements:**
M. J. Copley, G. F. Zellhoefer, and C. S. Marvel, J. Am. Chem. Soc. **61**, 3550–2 (1939).

**Variables:**
$T$/K=305

**Prepared By:**
V. P. Sazonov

**Experimental Data**
Solubility of dichlorofluoromethane (2) in nitrobutane (1)

| $t$/°C | $T$/K (compiler) | $g_2/100\,g_1$ | $100\,w_2$ (compiler) | $x_2$ (compiler) |
|---|---|---|---|---|
| 32.2 | 305.4 | 78.0 | 43.8 | 0.438 |

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The procedure followed in making the solubility measurements described in Zellhoefer.[1] No experimental details given.

**Source and Purity of Materials:**
(1) Source not specified; purity not specified; purified by distillation.
(2) Source not specified; purity not specified.

**Estimated Error:**
Solubility: reproducible to within 1%.

**References:**
[1]G. F. Zellhoefer, Ind. Eng. Chem. **37**, 584 (1939).

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