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DIPPR Project 882: Transport Properties and Related Thermodynamic Data for Binary Mixtures[1]

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DIPPR Project 882 was organized to develop a computerized databank of selected and evaluated physical, thermodynamic, and transport properties for mixtures of primarily organic compounds. The properties include: liquid viscosities, liquid thermal conductivities, mutual diffusion coefficients, excess volumes and densities, surface tensions, critical temperatures, critical pressures and densities, and solubilities of sparingly soluble organic compounds. The collection is *not* complete. It is estimated that the complete collection covers about 90% of the mixture classes, contains about 85% of the binary systems published, references about 80% of the data sources, and is a repository for about 85% of all the data published (these estimates exclude density and solubility where the coverage was not intended to be comprehensive). Exhaustive literature searches were made. The data from the original literature were assessed and differences from the pure component values derived from the DIPPR Project 801 and other reliable evaluated data sources for pure compounds were noted. In cases where the differences were excessive, the data sets were rejected. The total collection consists of about 2140 mixture/property pairs covering 361 mixture classes. The results of the project are distributed as five books in the series *Transport Properties and Related Thermodynamic Data of Binary Mixtures* published by the American Institute of Chemical Engineers and in electronic form as the *DIPMIX Database on Transport Properties and Related*

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Thermodynamic Data for Binary Mixtures distributed by the Thermodynamics Research Center.

KEY WORDS: critical properties; data bank; density; diffusion coefficients; evaluated data; organic mixtures; solubility; surface tension; thermal conductivity; viscosity.

1. INTRODUCTION

1.1. Scope of Work

The Design Institute for Physical Property Data, DIPPR,[6] of the American Institute of Chemical Engineers sponsored *Project* 882: *Evaluated Data on Mixtures* from 1988 to 1996 at the Thermodynamics Research Center (TRC), in order to satisfy industrial needs for accurate and comprehensive physical property data for mixtures. The emphasis was on transport properties (viscosity, thermal conductivity, and diffusion coefficient), liquid property data (solubility in organic, and aqueous solvents, excess volume, mixture density, and surface tension), and process design data (mixture critical properties). The properties chosen were those that were not well covered for mixtures by other data projects in existence at the inception of this project. TRC established procedures to locate, acquire, assess, enter, and corroborate the available literature data. In addition, software was developed for checking the consistency of the original and derived data. After review and incorporation of suggestions by Technical Steering Committee members, the results were released to the sponsors for proprietary use for one year before the data were released to the public.

The first release of data to the sponsors was in June 1991 and consisted of data for 130 mixture/property binary-mixture tables with 309 data sets. These tables covered binary mixtures from the following combinations of chemical classes: alcohols + water, alcohols + hydrocarbons, organic acids + water, and organic acids + hydrocarbons. The second release in November 1991 contained an additional 376 mixture/property tables with 554 data sets covering the above mixtures and the following additional classes: heavy hydrocarbons + light hydrocarbons, nitrogen, and hydrogen, aldehydes and ketones + water, and amines + water. The third release in November 1992 contained an additional 447 mixture/property tables with a total of 579 data sets. The emphasis was on polyalcohols + water,

[6] DIPPR is the registered trademark of the Design Institute for Physical Property Data, under the American Institute of Chemical Engineers.

alkanolamines + water, binary mixtures of C^1 and C^2 halogenated compounds, mixtures containing sulfur compounds, and aromatic fused ring compounds + hydrocarbons. The fourth and fifth releases were a combined release, which was initially made available to the sponsors in October 1993. This consisted of an additional 567 mixture/property tables with a total of 857 data sets. Many more classes of compounds were included in this release. The main emphasis was on mixtures of *n*-alcohols, alkanes, cycloalkanes, ethers, and aromatic alcohols + *n*-alkybenzenes, amides, ketones, and aminocarboxylic acids + inorganic compounds (including light gases), and mixtures containing multifunctional groups. The sixth release was made available to the project sponsors in Fall 1994 and consisted of 399 mixture/property pairs with a total of 516 data sets. The following classes were emphasized: alkyl carbonates + hydrocarbons, ethers + alcohols, esters, alcohols, and acids + esters, acids + aldehydes, and various mixtures of halogenated compounds of interest to new refrigerant technology. The seventh release was issued to the sponsors in two parts, release 7 was issued in Fall 1995, and release 7A was issued in Spring 1996 with a combined total of 489 mixture/property pairs consisting of 520 data sets. The emphasis on this release was to cover the recent literature and to make a more complete coverage of the mixture classes considered previously with an emphasis on properties that were underrepresented in the earlier releases.

1.2. Modes of Distribution

The books are published by AIChE under the title *Transport Properties and Related Thermodynamic Data of Binary Mixtures* in five parts. Part 1, containing 459 mixture/property tables, was published in 1993. Part 2, containing an additional 445 mixture/property tables, was published in 1994. Part 3, containing 567 mixture/property tables, was published in 1996 and Part 4, containing 886 mixture/property tables, was published in 1997. Part 5, which contains a comprehensive index to all the data tables in the first four parts, was published in 1998. After Parts 1 and 2 were published, certain errors in the tables were found. The corrected tables are included in Part 3. An example of the tables is given in Fig. 1. Additional features of Parts 3 and 4 are the inclusion of references to measurements which were considered to be of poor quality and were rejected from further analysis. Additionally, comments are given when the differences between the pure component property values and those values calculated from either the DIPPR 801 project equations or fixed values or from other recognized evaluated data sources were considered to be relatively large but not large enough to warrant rejection. In general, the guideline for

Dichlorodifluoromethane + 1,1,1,2-Tetrafluoroethane: Viscosity

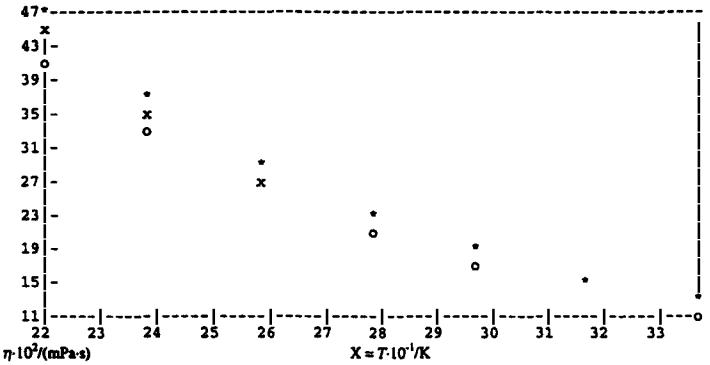
Source: Khalaidzhi, V. N.; Geller, V. Z.; Zaporozhan, G. V.; Inzh.-Fiz. Zh., 55(4), 620-624(1988)

Substance	Label	Formula	CASRN	Purity
Dichlorodifluoromethane	B	CCl_2F_2	75-71-8	pt;sx;ns;99.5w%,nc
1,1,1,2-Tetrafluoroethane	A	$C_2H_2F_4$	811-97-2	pt;sx;ns;99.3w%,nc

Variable	Symbol	Units	Imprecision	Inaccuracy
Temperature	T	K	0.1	0.2
Composition	x_B	molf	0.01	0.02
Viscosity	η	mPa·s	0.04 η	0.06 η

The system was in vapor liquid equilbrium. The pressures were found for a range of 0.1-20 MPa.

x_B =	0.21	0.54	0.72		0.21	0.54	0.72
T	η	η	η	T	η	η	η
220.	0.406	0.435	0.452	300.	0.161	0.168	0.177
240.	0.318	0.336	0.355	320.	0.129	0.134	0.142
260.	0.251	0.266	0.280	340.	0.105	0.108	0.115
280.	0.200	0.210	0.221				



$Y = \eta \cdot 10^2/(mPa \cdot s)$ $X = T \cdot 10^{-1}/K$

o, $x_B = 0.210$ molf; x, $x_B = 0.540$ molf; *, $x_B = 0.720$ molf

Carbon tetrachloride + Methanol: Viscosity

Source: Bamelis, P.; Huyskens, P.; Meeussen, E.; J. Chim. Phys. Phys. Chim. Biol., 62, 158-170(1965)

Substance	Label	Formula	CASRN	Purity
Carbon tetrachloride	A	CCl_4	56-23-5	pt;cm;dc,fd;99.7m%,gs
Methanol	B	CH_4O	67-56-1	pt;cm;dc,fd;99.8m%,gs

Variable	Symbol	Units	Imprecision	Inaccuracy
Temperature	T	K	0.05	0.1
Pressure	P	MPa	0.0002	0.002
Composition	x_B	molf	0.0002	0.0005
Viscosity	η	mPa·s	0.001 η	0.003 η

$P = 0.101$

T =	298.15	308.15	318.15	328.15		298.15	308.15	318.15	328.15
x_B	η	η	η	η	x_B	η	η	η	η
1.0000	0.545	0.476	0.417	0.366	0.4226	0.842	0.724	0.630	0.553
0.9616	0.577	0.502	0.440	0.385	0.2547	0.857	0.738	0.643	0.565
0.9029	0.626	0.543	0.476	0.415	0.1063	0.865	0.749	0.657	0.574
0.7853	0.719	0.619	0.537	0.466	0.0886	0.869	0.755	0.670	0.584
0.6934	0.770	0.656	0.570	0.496	0.0708	0.871	0.756	0.664	0.586
0.6107	0.807	0.691	0.598	0.518	0.0367	0.877	0.764	0.672	0.595
0.5618	0.815	0.700	0.607	0.528	0.0000	0.900	0.785	0.692	0.617
0.4787	0.839	0.720	0.623	0.541					

Fig. 1. Sample tables from Handbook Part 4.

making such comments was when the publication reported differences from the evaluated data sources greater than the following: critical temperature, 1 K; critical pressure, 0.05 MPa; critical volume, 8%; density, 0.5%; surface tension, 1.5%; thermal conductivity, 5.0%; and viscosity, 3.0%;

The database that is distributed by TRC as the DIPMIX Database on Transport Properties and Related Thermodynamic Data for Binary Mixtures contains all the data released to the public. The database employs LogicBase, a database management program written at Shell Development Company using the Phar Lap DOS-Extender. DIPMIX provides the user a convenient user-friendly way to access the mixture physical property data. A User's Manual provides the necessary information to install as well as successfully query and retrieve data from DIPMIX. This database has powerful search and statistical report capabilities.

2. DATA PROCESSING

2.1. Literature Search and Maintenance of Literature Files

After establishing the general class of mixtures to be covered in a particular literature search, specific compounds within these classes were identified and a detailed search for references on the selected properties was made using the printed version of Chemicals Abstracts. The printed Chemical Abstracts were used, as the electronic version does not cover years before 1968. Additionally, it was found that the electronic searching produced too many spurious hits. The compounds chosen included all of those in the particular class that had been evaluated in the DIPPR Project 801 as well as other compounds for which there are known significant amounts of data. In subsequent searches for each compound chosen, all papers with data that had the substance as a component and had properties pertinent to this project were put into the evaluation list in order to avoid searching more than one time for a selected substance name. This process gleaned all papers for any mixture involving the chosen substance and avoided having to visually rescan the literature for each different binary mixture containing the chosen compound. To reduce ultimate costs, this philosophy of capturing any information that may be at all pertinent to the project when such information was encountered in diverse materials was maintained throughout the efforts of literature retrieval, off-line evaluation, and data entry. In addition to the Chemical Abstracts (CA) searches, various bibliographies were searched for relevant data on the selected mixtures; these were used in initial searches to locate the sources of the data that were ultimately evaluated by inspection of the original journal article.

All issues of *J. Chem. Eng. Data* and *J. Chem. Thermodyn.* were searched for relevant articles. Current literature was also visually scanned for any data within the scope of this project as a part of the routine operations of TRC. After a candidate journal article had been identified for retrieval and evaluation, subsequent processing of this reference was recorded and tracked with a computer filing system to avoid duplication in both retrieving abstracts and in making copies of journal articles. The acquired reprints of journal articles were classified into the following categories for filing:

(1) data to be evaluated now,

(2) data to be entered,

(3) data to be evaluated at a later date,

(4) data entered and paper contains secondary references to be obtained,

(5) data entered and secondary references obtained,

(6) review papers and papers containing secondary references but no data, and

(7) cited secondary references containing neither data nor relevant references.

Papers in (1) were assessed as soon as possible after receipt and transferred to (2) or (3). After data entry, if secondary references were cited for relevant properties of any mixture, the paper was transferred to (4). When all secondary references were obtained, the paper in (4) was transferred to the completed section (5). Papers in (6) become a part of the body of intensive sources for frequent visual rescanning. Category (7) was maintained to avoid repetitious consideration of such references; a dismaying number of references not containing pertinent information is often cited with implications to the contrary.

The processing method chosen for the literature retrieval and off-line evaluation evolved from trying some methods that proved to be inefficient. Our initial searches using CA On-line were expensive and inefficient for the following reasons:

(1) repeat finding of same abstract,

(2) new searches required for different mixtures sets, and

(3) many hits were irrelevant and formats for visual review were cumbersome, i.e., large printouts or extensive scrolling.

Using the hard copy from decennial, pentennial, and annual indexes were found to be much more efficient because

(1) for a particular compound all relevant properties of its mixtures within the scope of this project were visually scanned at one time,

(2) hard copies could be searched and marked up without need for a computer terminal, and

(3) all CA hard copies were indexed and stored by compound.

2.2. Data Assessments and Entry Preparations

The original journal articles were reviewed to determine the quality of the data. For papers containing data under current purview of the DIPPR 882 project, all relevant data in each paper, including mixtures that are not under current purview, were assessed. Estimates of the measurement precision and the accuracy of the values for each variable, for example (T, P, x, viscosity), associated with the data were expressed as either constants or equations. In exceptional cases, imprecisions for individual data points were recorded with the body of the reported data. Assessments of the purity of the substances contained in the mixtures were recorded following the TRC Source database format. The purity assessments were used to place subjective confidence upon the data. Only in the rare instances where the nature and concentration of impurities were given could quantitative use be made of the purity information. In many instances only a small portion of the foregoing information was explicitly recorded in the original papers and judgments had to be made based upon prior personal experience in both making experimental measurements and from evaluating literature data. Evaluation of data published in the future could be greatly eased by ensuring that the authors present such information fully in an easily identifiable form.

The assessment sheet that was developed provided the auxiliary information and instructions for entering data directly from the reprint without manual transcription to data forms. The formats were chosen to minimize the preparations required for data entry, the instructions required for training data entry personnel, and the key strokes required to enter the data. Additional details of the formats used are given in a paper by Gammon et al. [1].

Upon completion of entry of information from a selected reference, the information was checked to rectify entry and format errors. The full

literature citation from the bibliographic data file was returned for comparison with that on the reprint. It was then determined if the compound names were in an extensive file containing CAS registry numbers and synonyms and, if not, an error message was issued to permit spelling checks. Compound names that presented persistent problems were automatically placed in a special file for subsequent examination by a nomenclature expert who made the necessary revisions in the master file of compounds. The files were also checked to ensure data of the proper dimensionality had been entered and that there were no problems in the formats of the records; where there were problems, explicit error messages were issued describing the entry deficiency.

Unit conversions and simple data transformations were accomplished with table lookups for unit conversion factors and by algebraic manipulation of the data. As an element of the conversion process, the values were tested to see if they were within reasonable physical limits. Where molecular weights were required, they were determined from molecular formulas in the list of compound names and Registry numbers. The requisite data from recognized evaluated data [2–9] were used for testing zero mole fraction results and for possible data renormalization.

If the difference between reliable values from these sources also exceeded specified limits, the sets were rejected. If the discrepancies were close to the limits, a warning note was given with the table. Data with a wide variety of tabular formats and numerical ranges were displayed graphically with a special program developed at TRC. The output from this program formed the basis for the preparation of the book. For Parts 1 and 2, a complex program converted this output into a QUIC file for printing on a QMS laser printer. Parts 3 and 4 were prepared from the output using specially developed Word Macros.

3. CONCLUSIONS

The aim of this project was to supply industry with their needs for evaluated property data for transport and thermodynamic properties for mixtures. The total collection consisting of approximately 2142 mixture/property pairs, covering 361 mixture classes, adds substantially to the body of available evaluated property data. It is estimated that the complete collection covers about 95% of the possible mixture classes, contains about 85% of the binary systems published, about 80% of the references, and 85% of all the data published. These estimates do not include property values for density and solubility where the coverage was never intended to be comprehensive. This database provides a sufficiently wide range of mixture types for the various properties to allow an exhaustive test of the

existing correlating equations and present predictive procedures, and the existence of the database should encourage the development of better prediction methods.

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