OPTIMIZING SOLVENT SELECTION FOR SEPARATION AND REACTION

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OPTIMIZING SOLVENT SELECTION FOR

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For my grandpa, Cecil John Smith

He knew the value of a good education.

For Kimberly

For all her love, devotion, and patience

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SUMMARY

Solvent selection is an important factor in chemical process efficiency, profitability, and environmental impact. Prediction of solvent phase behavior will allow for the identification of novel solvent systems that could offer some economic or environmental advantage.

A modified cohesive energy density model is used to predict the solid-liquid-equilibria for multifunctional solids in pure and mixed solvents for rapid identification of process solvents for design of crystallization processes. Some solubility data at several temperatures are also measured to further test the general applicability of the model.

Gas-expanded liquids have potential environmentally advantageous applications as pressure tunable solvents for homogeneous and heterogeneous catalytic reactions and as novel solvent media for anti-solvent crystallizations. The phase behavior of some carbon dioxide/organic binary systems is measured to provide basic process design information. Solvent selection is also an important factor in the anti-solvent precipitation of solid compounds. The influence of organic solvent on the solid-liquid equilibria for two solid pharmaceutical compounds in several carbon dioxide expanded solvents is explored. A novel solvent system is also developed that allows for homogeneous catalytic reaction and subsequent catalyst sequestration by using carbon dioxide as a "miscibility switch". The fundamental biphasic solution behavior of some polar organics with water and carbon dioxide are investigated.

CHAPTER I

INTRODUCTION

Several important issues confront the process development engineer in the chemical industry. While economic profitability is the cornerstone of any viable process, there is a balance between the optimization of the most efficient process and the potential environmental effect. Faced with the increasing environmental legislation, methods to identify alternative solvents with lower environmental impact and reduced waste production over traditional solvents have received much attention. Supercritical fluids is one alternative solvent class that have been the focus of research for the past 25 years for many applications, including the extraction of natural compounds and as pressure tunable reaction media. Other more benign solvent systems, including gas-expanded liquids, ionic-liquids, and near critical solvents have also been recently been investigated.

With the growing number of pharmaceutical and other biologically active molecules being investigated and produced, a method for the prediction of these multi-functional solids is needed. In Chapter II, a cohesive energy density model is used for the correlation and prediction of infinite dilution activity coefficients of solid compounds in pure and mixed solvents. Originally developed for the prediction of monofunctional liquid solvents, the model is reexamined and further extended for the prediction of solid solubilities with only a minimal amount of experimental data. The MOSCED (MOdified

Separation of Cohesive Energy Density) model is found to perform very well for many solid compounds, including some promising results in aqueous organic mixed solvents. In Chapter III, the solubilities of some solid pharmaceutical precursors in a variety of organic solvents and mixed organic solvents are measured to purposefully demonstrate specific interactions in solution, and realize the potential of the modeling effort.

Gas-expanded liquids, that is, a liquid solvent with up to 90% dissolved gas, are unique solvent mixtures that replace a portion of the organic solvent with a more benign gas, like carbon dioxide. They have been used as solvent media for heterogeneous and homogeneous reactions; and because the solvent power of the liquid can be easily controlled with pressure, many anti-solvent crystallization processes have been studied to control the morphology and size of the particle precipitate. In Chapter IV, the high pressure vapor-liquid equilibria of several carbon dioxide + organic solvent binary mixtures are measured with a quick and facile technique, and some insight is gained into the intermolecular interactions of carbon dioxide in solution.

For reactions involving permanent gases (H_2, CO, O_2) the complete miscibility of carbon dioxide with gaseous reactants can remove phase boundaries and eliminate mass transfer limitations. In gas expanded liquids, the solubility of the reactive gases is found to be greater than in pure liquid solvents. In Chapter V, the oxidation of 2-propanol to acetone in the presence of oxygen is considered as a model reaction system to investigate the solubility of oxygen in the carbon dioxide-expanded liquid. The high pressure vapor-liquid equilibrium of argon + carbon dioxide + 2-propanol is studied across a pressure range, indicating an improvement in the relative reactant concentration ratios, and thus

potentially enhancing the rate of reaction. Product formation is also found to affect the number of phases and the solubility of reactants in the liquid phase.

In an effort to reduce waste and byproduct generation, much effort has been focused on improving the rate and selectivity of homogeneous catalytic systems. However, difficulties in catalyst recovery and cost of recovery limit the use of some highly active catalysts, and often cheaper, less toxic, and less active catalysts are used instead, and are left in a waste stream or in the final product. Effective immobilization of organometallic catalysts can be achieved by using a water soluble catalyst in a water/organic biphasic system. By introducing a two phase system, severe mass transport limitations are present, especially if the reactant is sparingly soluble in the aqueous phase. In Chapter VI, a novel solvent system is explored that will improve the solubility of hydrophobic organic reactants in an aqueous phase with the catalyst, and subsequent addition of carbon dioxide will act as an anti-solvent and create two liquid phases. After CO_2-induced phase separation, the catalyst-rich aqueous phase and the product-rich organic phase can be easily separated and the catalyst recycled. This is an example of CO_2 as a "miscibility switch", whereby a homogeneous reaction is coupled with a heterogeneous separation. The high pressure liquid-liquid equilibria of three polar organic compounds with water and carbon dioxide are measured at several temperatures to establish the pressures required for sufficient phase purification.

Micronization of pharmaceutical compounds from supercritical or gas-expanded liquids allow for better control of size and morphology of the particles formed. The choice of organic solvent is a key factor in the resulting particle characteristics in gas

anti-solvent processing. The choice of solvent has a large effect on the optimum process pressure, the equilibrium solubility and other process design parameters. In Chapter VII, the solid-liquid equilibria of two model pharmaceutical compounds in several mixtures of carbon dioxide with organic solvents are investigated. Some insight into the local solvation phenomena is gained, and the predictive capabilities of the MOSCED model as a solvent selection guide is further explored for these high pressure systems.

Finally, Chapter VIII summarizes the implications of this work and discusses some areas are recommend for further research. This includes a potential modification of the MOSCED model to account for longer range ionic interactions, and for polymeric systems. Other systems that may exhibit carbon dioxide induced phase separation for catalyst sequestration of put forward. Some industrially relevant reactions are suggested that may benefit from the presence of a gas-expanded liquid.

CHAPTER II

PREDICTION OF SOLID SOLUBILITY IN PURE AND MIXED NON-ELECTROLYTE SOLVENTS

Introduction

Quantitative estimation of multi-component phase equilibria is important for the design of many chemical processes. Limiting activity coefficients (γ^{∞}) are most useful in characterizing phase equilibria, as they truly represent unlike-pair interactions in solution. There are a several reliable methods for measurement of γ^{∞} (Eckert, Newman et al. 1981; Eckert and Sherman 1996), and a number of estimation techniques (Fredenslund, Gmehling et al. 1977; Tochigi, Minami et al. 1977; Thomas and Eckert 1984; Weidlich and Gmehling 1987). Used in combination with a general free energy model, such as the Wilson (Wilson 1964), NRTL (Renon and Prausnitz 1968), or UNIQUAC (Prausnitz, Lichtenthaler et al. 1986), they can be applied to the estimation of multi-component phase equilibria. Often there is little mixture data available for a given system to correlate the necessary interaction parameters for the activity coefficient model and some type of prediction is necessary to facilitate the process design. In particular, for the design of crystallization processes the necessary solid-liquid equilibrium for a wide range of solvents is not available and a predictive method for solubility in pure and mixed solvents would be beneficial for optimum solvent selection. A useful technique for the estimation

of γ^{∞} is the UNIFAC method, but it is often limited in that it does not have any explicit representation of specific interactions, such as hydrogen bonds, and often performs less well for multi-functional molecules. In this chapter, the MOSCED model, which specifically characterizes specific interactions, is reevaluated and is applied to the prediction of the solubility of multi-functional solid compounds, i.e. pharmaceutical and pharmaceutical precursors.

The classic estimation technique for γ^{∞} and perhaps the most intuitively appealing methods at predicting activity coefficients is the regular solution theory (RST) (Hildebrand and Scott 1950). This theory extends the concept of "like dissolves like" into a useful equation approximating the energy of a compound into a cohesive energy density. This model is most applicable to non-polar, non-associating solvent systems and performs poorly for associated and solvating systems. One of the most obvious limitations of RST is the inability to predict negative deviations from ideality ($\gamma<1$). An extension of RST that is widely used in industry is the Hansen model (Hansen 1967; Hansen 2000), which divides the regular solution solubility parameter into three parameters accounting for dispersion, dipolarity, and hydrogen bonding nature of a compound. The parameters from this model have been shown to be somewhat useful predicting solubility behavior, but may perform poorly for associated and solvating systems, as it too cannot predict negative deviations. This is a serious limitation of the model, as one frequently seeks specific solvation for separation processes.

An alternative approach to estimation of activity coefficients is a group-contribution method. The Universal Functional Activity Coefficient (UNIFAC) model

(Fredenslund, Jones et al. 1975) and modified UNIFAC (Weidlich and Gmehling 1987) has been used to predict all types of phase equilibria to some degree of success. The model assumes that each functional group has a specific interaction energy with every other functional group; in order to quantify the interaction parameters experimental data must be available for every functional group pair. The UNIFAC model has been used to predict solubility data for solid compounds with mixed success (Lohmann, Röpke et al. 1998; Ahlers, Lohmann et al. 1999; Lohmann and Gmehling 2001). Many predictions of solid compounds are not possible because of missing interaction parameters or missing functional groups.

Several models based upon the concept of differences in cohesive energy density for correlating infinite dilution activity coefficients have been proposed in the literature (Thomas and Eckert 1984; Howell, Karachewski et al. 1989; Hait, Liotta et al. 1993). In the model by Hait et al., all of the adjustable parameters per compound are predicted by empirical equations for each functional family that relate solvatochromic parameters to model parameters. This severely limits predictions for multi-functional compounds, common to many solids, which do not fit into a distinct family, and generally the solvatochromic parameters for solids are unavailable.

Of these models the Modified Separation of Cohesive Energy Density or MOSCED model has been shown to be the most quantitative at correlating and predicting infinite dilution activity coefficients (Thomas and Eckert 1984). The prediction of activity coefficients at infinite dilution simplifies the modeling effort by only considering the interactions of one solute molecule in the solvent thus reducing the number of

interaction energies that must be considered and also removing the complication of the composition dependency of the activity coefficients. Eckert and Schreiber (Schreiber and Eckert 1971) have shown that VLE can be accurately predicted from activity coefficient model parameters reduced from infinite dilution activity coefficient data. For multifunctional solids, the MOSCED model seems an appropriate choice for predicting solubility because of the whole molecule approach. The model can effectively describe compounds with up to four parameters that can be applied to any solvent with available parameters.

The increase in the available literature data for γ^{∞} in the last two decades has prompted a re-examination and new regression of parameters for the MOSCED model. In this study, the MOSCED model was used to correlate 6441 γ^{∞} data points for 130 solvents to an absolute average deviation of 10.6% with one to four adjustable parameters for each solvent. The ability of the MOSCED model to correlate parameters for solid compounds for prediction of solid solubility is examined and compared to the performance of the UNIFAC model. The MOSCED model is also extended to prediction of gas solubility in liquid solvents.

MOSCED Model Reevaluation

Since the initial formulation of the MOSCED model the amount and quality of infinite dilution activity coefficient data has increased. Several new techniques have been developed that allowed for faster determination of activity coefficient data. These include head space gas chromatographic techniques (Park, Hussam et al. 1987; Li and

Carr 1993; Dallas and Carr 1994; Asprion, Hasse et al. 1998; Castells, Eikens et al. 2000), dew point techniques (Trampe and Eckert 1993), and others of which there are several excellent reviews (Eckert and Sherman 1996; Sandler 1996). The first step in the re-examination of the MOSCED model was collecting the available literature data since the original formulation. The old data set was heavily weighted to nonpolar alkane systems having been the most investigated in the literature. Since then, infinite dilution activity coefficient data for a larger range of organic compound structures and functionalities have been reported, including the data measured by Gmehling (Schiller and Gmehling 1992; Gruber, Langenheim et al. 1997; Möllmann and Gmehling 1997; Gruber, Langenheim et al. 1998; Gruber, Topphoff et al. 1998; Gruber, Topphoff et al. 1998; Krummen, Letcher et al. 2000; Topphoff, Gruber et al. 2000; Krummen, Letcher et al. 2002) as well as published literature data since the DECHEMA publication (Gmehling, Onken et al. 1977). Additionally, the available VLE data from the International Data Series (TRC 1973) were used to estimate infinite dilution activity coefficients using the Wilson activity coefficient model. The data set was vetted for suspect points by comparison with other existing data, either with the same system if available or with a homologous series. In addition, if data was available at multiple temperatures, a plot of the data versus inverse temperature was useful in identifying suspect data. When a preponderance of data from a single reference source were deemed suspect, the entire reference was removed from the database. In general the data measured using the liquid chromatography technique were removed from the database because of the disagreement with the other existing data and known experimental

Table 2-1. Parameters for the MOSCED model at 20°C. Parameters λ, τ, α, and β are in units of $(J/cm^3)^{1/2}$.

Compound	v (cm^3/mol)	λ	τ	q	α	β
propane	75.7	13.10	0.00	1.00	0.00	0.00
butane	96.5	13.70	0.00	1.00	0.00	0.00
pentane	116.0	14.40	0.00	1.00	0.00	0.00
isopentane	117.1	13.87	0.00	1.00	0.00	0.00
cyclopentane	94.6	16.55	0.00	1.00	0.00	0.00
hexane	131.4	14.90	0.00	1.00	0.00	0.00
cyclohexane	108.9	16.74	0.00	1.00	0.00	0.00
methylcyclopentane	113.0	16.10	0.00	1.00	0.00	0.00
3-methylpentane	130.4	14.68	0.00	1.00	0.00	0.00
2-methylpentane	132.9	14.40	0.00	1.00	0.00	0.00
2,3-dimethylbutane	131.2	14.30	0.00	1.00	0.00	0.00
2,2-dimethylbutane	133.7	13.77	0.00	1.00	0.00	0.00
heptane	147.0	15.20	0.00	1.00	0.00	0.00
methylcyclohexane	128.2	16.06	0.00	1.00	0.00	0.00
cycloheptane	121.7	17.20	0.00	1.00	0.00	0.00
3-methylhexane	146.4	14.95	0.00	1.00	0.00	0.00
2,2-dimethylpentane	148.9	14.26	0.00	1.00	0.00	0.00
2,4-dimethylpentane	150.0	14.29	0.00	1.00	0.00	0.00
2,3,4-trimethylpentane	159.5	14.94	0.00	1.00	0.00	0.00
octane	163.4	15.40	0.00	1.00	0.00	0.00
2,2,4-trimethylpentane	165.5	14.08	0.00	1.00	0.00	0.00
ethylcyclohexane	143.0	16.34	0.00	1.00	0.00	0.00
cyclooctane	134.9	17.41	0.00	1.00	0.00	0.00
2,5-dimethylhexane	165.6	14.74	0.00	1.00	0.00	0.00
nonane	179.6	15.60	0.00	1.00	0.00	0.00
decane	195.8	15.70	0.00	1.00	0.00	0.00
dodecane	228.6	16.00	0.00	1.00	0.00	0.00
tetradecane	261.3	16.10	0.00	1.00	0.00	0.00
hexadecane	294.2	16.20	0.00	1.00	0.00	0.00
squalane	526.1	14.49	0.00	1.00	0.00	0.00
1-pentene	110.3	14.64	0.25	0.90	0.00	0.24
1-hexene	125.8	15.23	0.22	0.93	0.00	0.29
1-octene	157.8	15.39	0.44	0.95	0.00	0.51

Compound	v (cm^3/mol)	λ	τ	**q**	α	β
alpha-pinene	159.0	17.32	0.15	0.95	0.00	1.30
benzene	89.5	16.71	3.95	0.90	0.63	2.24
toluene	106.7	16.61	3.22	0.90	0.57	2.23
p-xylene	123.9	16.06	2.70	0.90	0.27	1.87
ethylbenzene	122.9	16.78	2.98	0.90	0.23	1.83
isopropylbenzene	139.9	17.09	3.23	0.90	0.20	2.57
butylbenzene	156.6	17.10	2.51	0.90	0.10	1.83
methanol	40.6	14.43	3.77	1.00	17.43	14.49
ethanol	58.6	14.37	2.53	1.00	12.58	13.29
1-propanol	75.1	14.93	1.39	1.00	11.97	10.35
2-propanol	76.8	13.95	1.95	1.00	9.23	11.86
1-butanol	92.0	14.82	1.86	1.00	8.44	11.01
2-butanol	92.0	14.50	1.56	1.00	8.03	10.21
2-methyl-2-propanol	94.7	14.47	2.55	1.00	5.80	11.93
2-methyl-1-propanol	92.9	14.19	1.85	1.00	8.30	10.52
1-pentanol	108.5	15.25	1.46	1.00	8.10	9.51
1-hexanol	125.2	15.02	1.27	1.00	7.56	9.20
1-octanol	158.2	15.08	1.31	1.00	4.22	9.35
phenol	88.9	16.66	4.50	0.90	25.14	5.35
benzyl alcohol	103.8	16.56	5.03	1.00	15.01	6.69
m-cresol	105.0	17.86	4.16	0.90	27.15	2.17
2-ethoxyethanol	97.3	15.12	7.39	1.00	3.77	16.84
methyl acetate	79.8	13.59	7.54	1.00	0.00	8.38
ethyl acetate	98.6	14.51	5.74	1.00	0.00	7.25
propyl acetate	115.8	13.98	5.45	1.00	0.00	7.53
butyl acetate	132.0	15.22	4.16	1.00	0.00	6.40
benzyl acetate	142.9	16.17	6.84	0.90	0.54	5.53
methyl formate	62.1	18.79	8.29	1.00	0.37	8.62
ethyl benzoate	144.1	16.48	4.97	1.00	0.28	2.40
diethyl phthalate	199.7	16.33	6.14	1.00	1.07	7.81
acetone	73.8	13.71	8.30	1.00	0.00	11.14
2-butanone	90.2	14.74	6.64	1.00	0.00	9.70
2-pentanone	107.3	15.07	5.49	1.00	0.00	8.09
cyclohexanone	104.1	15.80	6.40	1.00	0.00	10.71
4-methyl-2-pentanone	125.8	15.27	4.71	1.00	0.00	6.34

Compound	v (cm^3/mol)	λ	τ	q	α	β
2-heptanone	140.7	14.72	4.20	1.00	0.00	6.08
1-phenyl-1-butanone	145.2	16.46	4.98	1.00	0.88	6.54
acetophenone	117.4	16.16	6.50	0.90	1.71	7.12
epsilon-caprolactone	106.8	16.42	9.65	1.00	0.43	13.06
dichloromethane	64.4	15.94	6.23	0.96	3.98	0.92
chloroform	80.5	15.61	4.50	0.96	5.80	0.12
carbon tetrachloride	97.1	16.54	1.82	1.01	1.25	0.64
1,1-dichloroethane	84.7	16.77	6.22	0.92	3.28	1.56
1,2-dichloroethane	79.4	16.60	6.58	0.94	2.42	1.34
1,1,1-trichloroethane	100.3	16.54	3.15	1.01	1.05	0.85
trichloroethylene	90.1	17.19	2.96	1.00	2.07	0.21
1-chlorobutane	105.1	15.49	3.38	1.00	0.11	1.17
chlorobenzene	102.3	16.72	4.17	0.89	0.00	2.50
bromoethane	75.3	15.72	4.41	1.00	0.22	1.56
bromobenzene	105.6	17.10	4.29	0.89	0.00	3.13
iodomethane	62.7	19.13	4.21	1.00	1.16	0.83
diiodomethane	81.0	21.90	5.19	1.00	2.40	2.08
iodoethane	93.6	17.39	3.58	1.00	0.51	1.96
acetonitrile	52.9	13.78	11.51	1.00	3.49	8.98
propanenitrile	70.9	14.95	9.82	1.00	1.08	6.83
butanenitrile	87.9	14.95	8.27	1.00	0.00	8.57
benzonitrile	103.0	15.43	8.21	0.90	0.15	7.41
glutaronitrile	95.8	15.12	12.59	1.00	3.76	9.11
nitromethane	54.1	13.48	12.44	1.00	4.07	4.01
nitroethane	72.0	14.68	9.96	1.00	1.19	4.72
1-nitropropane	89.5	15.17	8.62	1.00	0.28	5.83
2-nitropropane	90.6	14.60	8.30	1.00	0.55	3.43
nitrobenzene	102.7	16.06	8.23	0.90	0.98	3.29
DMF	77.4	15.95	9.51	1.00	1.22	22.65
N,N-dibutylformamide	182.0	15.99	5.02	1.00	0.24	14.07
N,N-dimethylacetamide	93.0	15.86	9.46	1.00	0.00	21.00
N,N-diethylacetamide	124.5	15.66	6.71	1.00	0.25	18.67
N-methylformamide	59.1	15.55	8.92	1.00	8.07	22.01
N-methylacetamide	76.9	16.22	5.90	1.00	5.28	23.58
N-Ethylacetamide	94.3	16.07	4.91	1.00	4.14	22.45

Compound	v (cm^3/mol)	λ	τ	**q**	α	β
aniline	91.6	16.51	9.41	0.90	6.51	6.34
2-Pyrrolidone	76.8	16.72	11.36	1.00	2.39	27.59
N-methylpyrrolidone	96.6	17.64	9.34	1.00	0.00	24.22
1-Ethylpyrrolidin-2-one	114.1	16.74	8.31	1.00	0.00	20.75
1,5-Dimethyl-2-pyrrolidinone	115.2	16.50	8.45	1.00	0.00	22.66
N-formylmorpholine	100.6	16.10	10.91	1.00	2.42	19.29
pyridine	80.9	16.39	6.13	0.90	1.61	14.93
2,6-dimethylpyridine	116.7	15.95	4.16	0.90	0.73	13.12
quinoline	118.5	16.84	5.96	0.90	2.17	12.10
sulfolane	95.3	16.49	12.16	1.00	1.36	13.52
DMSO	71.3	16.12	13.36	1.00	0.00	26.17
dioxane	85.7	16.96	6.72	1.00	0.00	10.39
tetrahydrofuran	81.9	15.78	4.41	1.00	0.00	10.43
diethyl ether	104.7	13.96	2.79	1.00	0.00	6.61
dipropyl ether	137.6	15.20	2.00	1.00	0.00	5.25
dibutyl ether	170.4	15.13	1.73	1.00	0.00	5.29
diisopropyl ether	141.8	14.72	1.90	1.00	0.00	6.39
methyl tert-butyl ether	119.9	15.17	2.48	1.00	0.00	7.40
anisole	109.2	16.54	5.63	0.90	0.75	3.93
tetraethylene glycol dimethyl ether	221.1	16.08	6.73	1.00	0.00	13.53
acetic acid	57.6	14.96	3.23	1.00	24.03	7.50
dimethyl carbonate	84.7	17.81	8.05	1.00	0.00	7.32
acetaldehyde	56.5	13.76	8.48	1.00	0.00	6.50
butanal	90.4	15.11	5.97	1.00	0.00	5.27
carbon disulfide	60.6	19.67	1.04	1.00	0.59	0.33
triethylamine	139.7	14.49	1.02	1.00	0.00	7.70
tributyl phosphate	345.0	15.05	4.87	1.00	0.00	14.06
water	36.0	10.58	10.48	1.00	52.78	15.86

Table 2-2. Absolute average % error in regressed activity coefficients for different classes of compounds: Nonpolar, polar aprotic, aromatic and halogenated, polar associated and water.

Solute	Solvent	MOSCED	UNIFAC
nonpolar	nonpolar	6.1 %	5.8 %
polar aprotic		11.8 %	12.6 %
aroma./halogen		8.3 %	13.9 %
associated		13.4 %	16.0 %
nonpolar	polar aprotic	10.6 %	14.9 %
polar aprotic		10.4 %	14.8 %
aroma./halogen		11.0 %	16.4 %
associated		13.3 %	21.1 %
nonpolar	aroma/halogen	7.6 %	14.4 %
polar aprotic		10.2 %	17.1 %
aroma./halogen		7.0 %	14.7 %
associated		13.5 %	21.4 %
nonpolar	associated	10.5 %	14.1 %
polar aprotic		8.9 %	23.3 %
aroma./halogen		11.5 %	11.7 %
associated		14.3 %	21.7 %
nonpolar	water	51.7 %	96.6 %
polar aprotic		59.5 %	54.2 %
aroma./halogen		29.9 %	172.1 %
associated		38.8 %	43.4 %

uncertainties in data measured by this technique. The database used to reevaluate/refit the MOSCED model was limited to 6441 data points for 130 organic solvents.

The parameters were regressed by minimizing the objective function in equation 2-1 and Powell algorithm (Press, Teukolsky et al. 1992).

$$O.F. = \left(\ln \gamma^{\infty}_{\text{exp}} - \ln \gamma^{\infty}_{\text{pred}}\right)^2 \qquad \text{Eq. 2-1}$$

The root mean squared error for ln γ^{∞} was 0.148. The overall average absolute deviation (AAD) for γ^{∞} was 10.6%, which is slightly larger than the original correlation where the dataset was roughly half the size. The parameters in units of $(J/cm^3)^{1/2}$ are shown in Table 2-1. The model is able to correlate accurately the data for the following classes of compounds: nonpolar, polar aprotic (dipolar and hydrogen bond accepting), aromatic/halogenated (large dispersion and slight hydrogen bond donating/accepting), and associated (dipolar and strong hydrogen bond donating/accepting). The AADs for the different classes are shown in Table 2-2. MOSCED performs best for nonpolar and aromatic/halogenated compounds with slightly higher errors for polar aprotic and associated compounds. UNIFAC is able to predict the dataset to an average error of 16.3% with the highest errors for systems with associated solvents and solutes. For the UNIFAC model the predictions for 2,6-dimethylpyridine, butanenitrile, and glutaronitrile are consistent outliers from the average deviation. For the case of 2,6-dimethylpyridine and butanenitrile, UNIFAC is unable to account properly for the chemical effect upon addition of methyl groups to pyridine and acetonitrile which are not consistent outliers form the average deviation. A plot of the experimental versus predicted values for MOSCED and UNIFAC are shown in Figure 2-1. The UNIFAC model in general tends

to under-predict the activity coefficients and some of the under-predicted points are strong outliers. The only outliers for the MOSCED prediction are for two points with activity coefficients less than 0.1. All experimental data with MOSCED and UNIFAC predictions and percent error are shown in Appendix E.

The form and parameters of the model were reexamined in light of the currently available data. The error and consistency (scatter) of data was found to be too large to make substantial changes in the model constants. Several reviews of the available infinite dilution activity coefficient data in the literature (Eckert and Sherman 1996; Sandler 1996) and my own review of the available data have shown this to be case. The constants of the model in the asymmetry parameter function, Flory-Huggins term, and in the parameter temperature dependency were found to be sufficient to give a quality fit. The compound parameters were refit to the existing data with some changes in the approach to finding the best set of parameters. The MOSCED model with all asymmetry parameters and temperature dependencies is shown in Table 2-3.

As with the original formulation of the MOSCED model upto five parameters are used to characterize the energy of interaction of a compound in solution. Of these parameters, chemical intuition is used to determine which parameters need to be fit for a given compound. We will discuss the significance of each parameter and the approach taken to arrive at the best set of compound parameters.

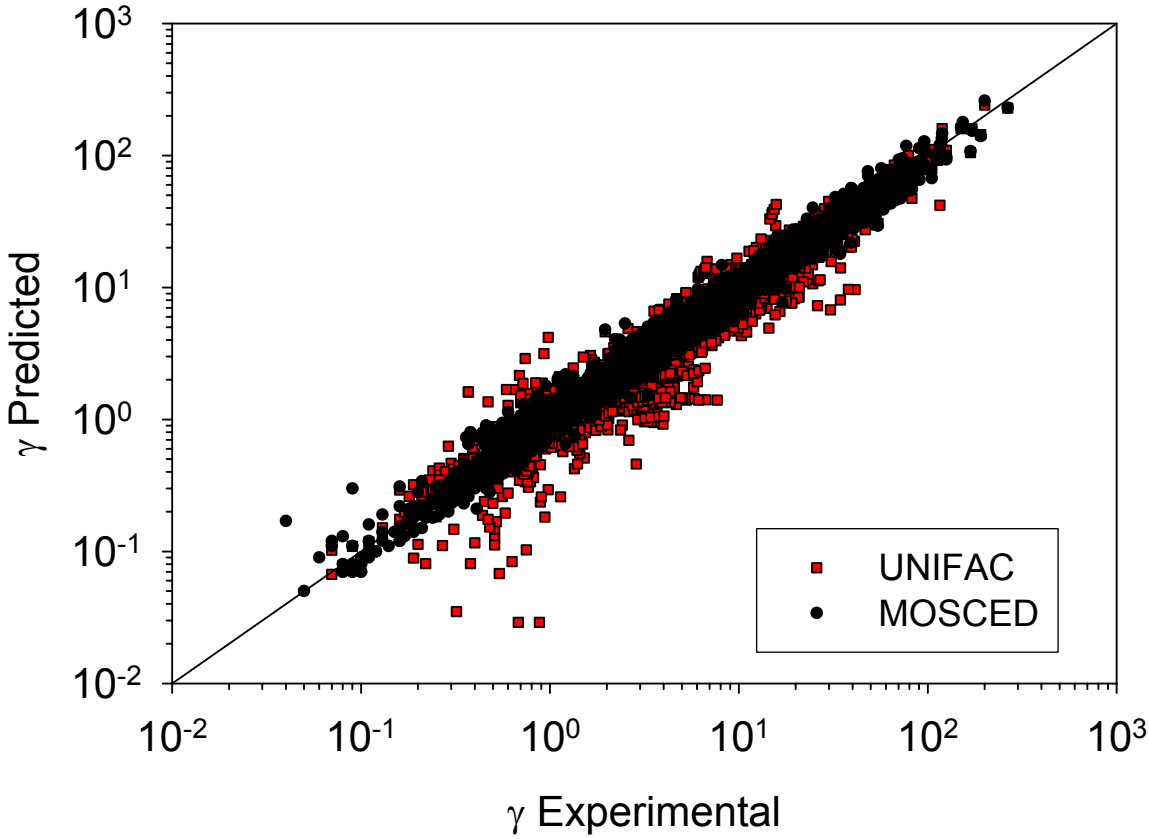

Figure 2-1. Experimental versus predicted values for both UNIFAC and MOSCED.

Table 2-3. MOSCED model.

$$\ln \gamma_2^{\infty} = \frac{v_2}{RT}\left[(\lambda_1 - \lambda_2)^2 + \frac{q_1^2 q_2^2 (\tau_1 - \tau_2)^2}{\psi_1} + \frac{(\alpha_1 - \alpha_2)(\beta_1 - \beta_2)}{\xi_1}\right] + d_{12}$$

$$d_{12} = \ln\left(\frac{v_2}{v_1}\right)^{aa} + 1 - \left(\frac{v_2}{v_1}\right)^{aa}$$

$$aa = 0.953 - 0.00968\left(\tau_2^2 + \alpha_2\beta_2\right)$$

$$\alpha_T, \beta_T = (\alpha_{293}, \beta_{293})\left(293/T\right)^{0.8} \qquad \tau_T = \tau_{293}\left(293/T\right)^{0.4}$$

$$\psi = POL + 0.011\alpha_T\beta_T$$

$$\xi = 0.68(POL - 1) + \left[3.24 - 2.4\exp\left(-0.023(\alpha_o\beta_o)^{1.5}\right)\right]^{(293/T)^2}$$

$$POL = q^4\left(1.15 - 1.15\exp\left(-0.02\tau_T^3\right)\right) + 1$$

Dispersion Parameter, λ. The initial formulation of the MOSCED model used two functions of the refractive index, one for non-aromatic and one for aromatic compounds, to give the value of the dispersion parameter. The original linear correlations for the dispersion parameter were found to be insufficient to fit the data for very polar and basic compounds like DMSO and NMP. No suitable correlation could be found that could represent the dispersion parameters for all classes of compounds. The original correlation is not suitable for finding dispersion parameters for solid compounds, for which values of the refractive index of the liquid are not available. In this refitting of parameters, the dispersion parameters were fit for each compound, with the exception of alkane compounds which were set to the value of the solubility parameter.

Polarity Parameter, τ. The polarity parameter is meant as a measure of the fixed dipole of a compound in solution. The original formulation used essentially a homomorph method, but this approach was not used in the refit, as it was not generally applicable to aromatic or branched carbon backbones or to multi-functional compounds. The values found for polar compounds are consistent with the gas phase dipole moment data with the τ for DMSO (3.96 D) being the largest at 13.36, lower for nitromethane (3.46 D) at 12.44, and less for acetone (2.88 D) at 8.30. No sufficiently quantitative correlation could be found that relates the dipole moment to the regressed value of τ, although there is an approximate linear correlation with the ratio of the dipole moment and the molar volume. 1,4-Dioxane is one example where the zero dipole moment in the gas phase is not in agreement with the expected more polar behavior in liquid solution.

The polarity parameter value of 6.72 is similar to that of the moderately polar 2-butanone. This disparity may be due to the chair-boat transitions of dioxane.

The same approximation for the temperature dependency of the polarity parameter was used, as shown in equation 2-2. A better function for the temperature dependency was attempted, but the limited accuracy and quantity of data across a large temperature range precluded changes.

$$\tau_T = \tau_{293}\left(293/T\right)^{0.4} \qquad \text{Eq. 2-2}$$

Induction Parameter, q. The induction parameter attempts to account for the dipole-induced dipole and induced dipole-induced dipole interactions that can occur in compounds with large dispersion (polarizability) parameters. For compounds with large dispersion parameters, namely aromatic and halogenated compounds, the increased interaction of the dispersion forces tends to lessen the dipolar interactions and thus the value of the induction parameter would be less than one. For aromatic compounds q is set to 0.9 and for halogenated compounds the polarity parameter is varied for best fit.

Acidity and Basicity Parameters, α and β. The acidity and basicity parameters account for specific interactions due primarily due to hydrogen bond formation through both association and solvation. As in the initial formulation the α parameter was kept at a value of zero unless deemed physically reasonable for that particular compound. The α also can account for the Lewis acidity as in the case of acetonitrile and nitromethane, where a non-negligible value of α is necessary to correlate the data. In the case of alcohols the values of α and β were allowed to correlated independent of each another

and were not forced to the same value. This resulted in better fits for the alcohols and a larger α parameter than the β parameter for short chain alcohols with the a parameter decreasing more rapidly with increasing carbon chain length so that at long chain lengths (1-octanol) the β parameter is larger than the α parameter. The β parameter is also able to capture the strongly basic nature of compounds like DMSO, DMF, and NMP with the largest correlated β values. The temperature dependency for the acidity/basicity parameters, as shown in equation 2-3, is the same as in the original model and was not altered for the same reasons as stated for the polarity parameter

$$\alpha_T, \beta_T = (\alpha_{293}, \beta_{293})\left(293/T\right)^{0.8} \qquad \text{Eq. 2-3}$$

Addition of Water Parameters. The magnitude and range of the infinite dilution activity coefficients for organics in water (10^{-1} to 10^{10}) are much larger than the other organic data. In addition, the variability/discrepancies in experimental data are much larger for aqueous systems than most other organic solvent data due to experimental difficulties (Sherman, Trampe et al. 1996). For these reasons the parameters for water were fit independent of the organic compound parameters. Using the molar volume of water (18 ml/mol) in the model resulted in a poor fit of the data and gave unreasonably low values for the activity coefficient of water in the organic solvent. The molar volume of water was treated as an adjustable parameter and the optimum value was found at a molar volume of 36 ml/mol. The extensive hydrogen bond network present in water could possibly cause water to act with a larger molar volume in solution. With this change, MOSCED is able to correlate the activity coefficients of organics in

water to 41.1% AAD, which is good considering the large range of values. As can be seen in Figure 2-2, plotting the UNIFAC and MOSCED predictions versus the experimental activity coefficients, UNIFAC exhibits some interesting behavior, exhibiting a large number of outliers that are offset from the best-fit line. The under-predicted outliers are mostly for nonpolar compounds. The MOSCED model does exhibit some outliers at the smaller activity coefficients, though it does not exhibit any systematic error for range of activity coefficients.

Estimation of Parameters

The addition of new solvents to the database can be most directly achieved by fitting experimentally determined activity coefficient data with all the interactions covered. This set of data would necessarily include data with a nonpolar, a mildly polar basic, a strongly polar basic, and a polar associated compound. It should be noted, there can be multiple solutions for the best fit parameters with a given set of data and care should be taken that the parameters match our intuitive sense of the compound and are consistent with other similar compounds either through a homologous series or a homomorphic series.

The cohesive energy density (c) is defined as specific energy of vaporization per molar volume of pure liquid and it is possible to relate the MOSCED parameters to the pure component heat of vaporization. The separation of cohesive energy concept, upon which the MOSCED model is based, directly relates the cohesive energy density to the model parameters by equation 2-4, in the same manner that the solubility parameter (δ) is

defined in the regular solution theory. Calculation of the MOSCED parameters from this equation is not possible because as pointed out by Thomas (Thomas and Eckert 1984),

$$c = \delta^2 = \lambda^2 + \tau^2 + \alpha\beta \qquad \text{Eq. 2-4}$$

the inaccuracies in the heat of vaporization measurements limit the calculation of the MOSCED parameters directly from the cohesive energy density. However, from the regressed MOSCED parameters a reasonable correlation with the enthalpy of vaporization is achieved. The optimum linear correlation of the pure component energy parameters with the experimental heat of vaporization is shown in equation 2-5, and a

$$c = \frac{\Delta H_{vap} - RT}{v} = 1.02\ \lambda^2 + 2.49\ \tau^2 + 3.07\ \alpha\beta \qquad \text{Eq. 2-5}$$

plot of the experimental versus the predicted values are shown in Figure 2-3. The one outlier from the correlation is for water, which is over-predicted because of the magnitude of parameters regressed for the hydrogen bond acidity and basicity (α = 52.8, β =15.9). This equation, while not of sufficient quality to be used as a constraint in regressing parameters for the MOSCED model, is useful as a guideline for establishing parameter values for new solvents.

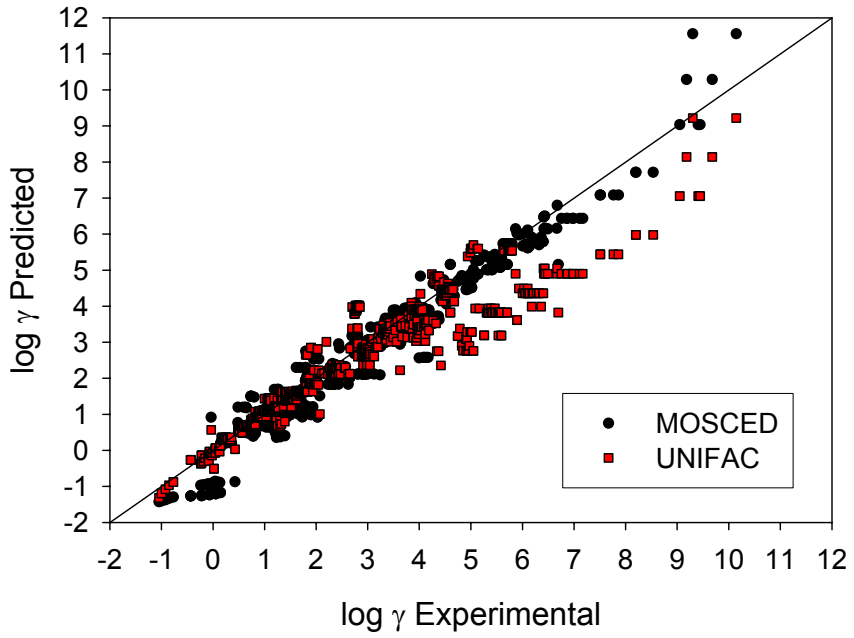

Figure 2-2. Experimental versus predicted of log of infinite dilution activity coefficients of organic compounds in water with both MOSCED and UNIFAC models.

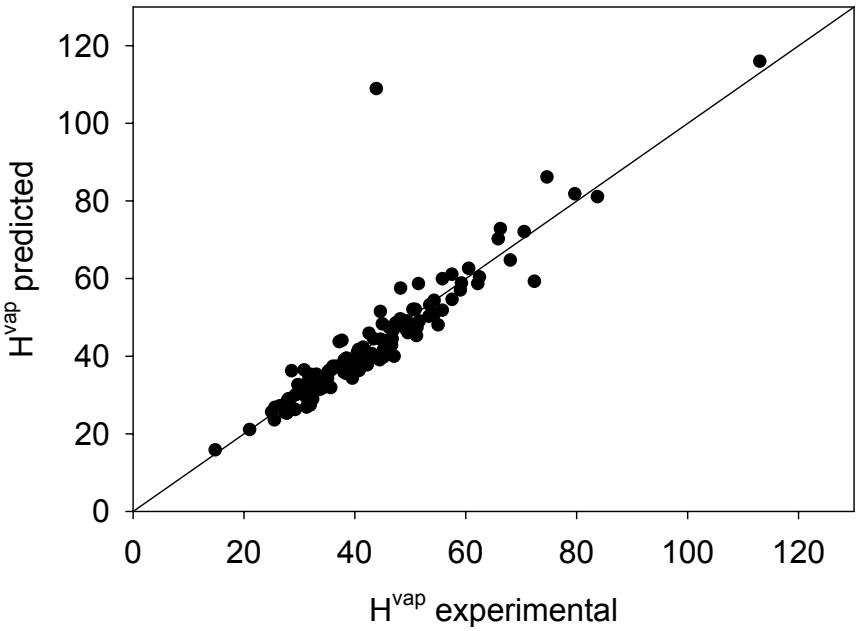

Figure 2-3. Enthalpy of vaporization predictions using linear correlation of MOSCED parameters.

Solid Solubility Modeling

The extension of the MOSCED model to predict activity coefficients for a saturated solution requires the calculation of the ideal solubility of the solid solute in the solvent. If one takes the standard state as the hypothetical sub-cooled liquid of the pure solid solute at the same temperature of the solution the solubility can be found from equation 2-6.

$$x^{ideal} = x_S \gamma_S = \exp\left[\frac{-\Delta H_{fus}}{RT_m}\left(\frac{T_m}{T} - 1\right) - \frac{\Delta C_p}{R}\left(\ln\frac{T_m}{T} - \frac{T_m}{T} + 1\right)\right] \qquad \text{Eq. 2-6}$$

where ΔH_{fus} is the enthalpy of fusion at the melting point temperature T_m, R is the universal gas constant, ΔC_p is the difference in heat capacity of the sub-cooled liquid and crystalline solute, γ_s is the activity coefficient of the solid in the solution, x_s is the equilibrium concentration in the solution, and x^{ideal} is the ideal solubility and is independent of the solvent. Equation 2-6 makes the following valid assumptions: the difference between the molar volume of the liquid solute and solid is negligible; the difference between the heat capacity is insensitive to temperature changes; and the triple point temperature is the same as the melting point temperature.

Although the heat capacity contribution to the overall solubility is small compared to the enthalpy of fusion term, its effect on the solubility can not be neglected especially for compounds with melting points far from the temperature of interest. For example, if the temperature of interest is 298 K and the melting point of the solid is 498 K, a ΔC_p of 10 J mol^{-1} K^{-1} will affect the ideal solubility by 20%. Also, if there is any change in crystalline structure during dissolution of the solid, the enthalpy of that polymorphic

transition must be added to correctly determine the ideal solubility. The ideal solubility could also be affected by the organic solvent in which it is dissolved, if those solvents change the crystal structure and thus the enthalpy of fusion or melting point temperature.

The infinite dilution activity coefficients of the solute in the liquid phase are calculated using MOSCED and interaction parameters for the g^E model are fit to the calculate γ^{∞}s. The mole fraction concentration of the solute in the liquid phase (x_S) and activity coefficient (γ_S) are found that satisfy the relationship in equation 8-2. The solid solute MOSCED parameters are found by the minimizing the sum of squared error in solubility between experimental and calculated values. The prediction made by the MOSCED model yields an activity coefficient value for both the dilute hypothetical sub-cooled liquid solute in the liquid solvent phase and the activity coefficient of the dilute liquid in the hypothetical sub-cooled liquid. Both activity coefficients are used to find the interaction parameters in the 2-parameter activity coefficient model. The solid solute phase in equilibrium with the saturated liquid solution is assumed to be pure solute and contain no liquid solvent; therefore the activity of the dilute liquid solvent in the sub-cooled liquid solute is only an artifact of the calculation technique.

To validate the ability of the MOSCED model to describe accurately solid-liquid equilibria, solubility data for a multifunctional solid solute in a variety of organic solvents are necessary. There are limited solubility data available in the literature for solids in a variety of organic solvents, mostly for polyaromatic compounds containing few functional groups, although there are some data available for pharmaceutical/agricultural compounds. From the available literature data five solid compounds were chosen that

reflect a variety of structure and functionality. Predictions were made with both the MOSCED and UNIFAC models.

For 26 solutes MOSCED parameters have been correlated from the available data in literature. Solutes selected were limited to those with data in a variety of solvents to allow for accurate parameterization and demonstration of the capabilities of the model. The regressed parameters are shown in Table 2-4 with the AAD% in prediction for the UNIFAC model for comparison. The UNIFAC model was able to correlate only 16 of the 26 solutes studied, because either necessary functional groups are missing or interaction parameters are not available. For all 26 solutes in this study the MOSCED model with the Wilson g^E model is able to correlate the 700 data points of solubility to an AAD% of 24.9%. MOSCED performs similarly to the UNIFAC model for polyaromatic hydrocarbons and is superior in predicting solubility of polar and multi-functional solid compounds. Tables of the experimental data with MOSCED and UNIFAC predictions are available in Appendix F.

The simplest molecule examined in this study is phenanthrene (T_m = 372.4 K, H_{fus} = 3934.8 cal/mol, ΔC_p = 3 cal/mol, T_{trans} = 339.2 K, H_{trans} = 312.4 cal/mol). The solubilities of phenanthrene in 37 organic solvents (Acree and Abraham 2001) were correlated with MOSCED and predicted with UNIFAC. The large dispersion term is expected for the polarizable π electrons in the poly-aromatic structure which can also act as a weak base which is reflected in the small β term. The large polarity term τ could possibly be attributed to the non-linear structure of phenanthrene. The UNIFAC model predicts the solubility to 37% absolute average deviation (AAD) and MOSCED is able to

correlate the data to 23.8% AAE. A plot of the experimental mole fraction versus the predicted mole fraction is shown in Figure 2-4, where a perfect prediction of the data is represented by the solid line.

The MOSCED model does not require extensive solubility data in order to parameterize a given solute. Solubility data for a small but chemically diverse solvent set is sufficient to describe the possible interactions that a given solute can experience in solution. For example, from the 37 available data points of phenanthrene solubility, we select 6 solvents that cover a range of functionality: hexane (non-polar), ethyl acetate (polar aprotic), 2-butanone (polar aprotic), acetonitrile (polar weak acid), ethanol (polar associated), and 2-propanol (polar associated). The best-fit parameters to this smaller data set results in some small changes in the values, with the dispersion increasing slightly to 18.93 from 18.48, the polarity decreasing to 5.16 from 5.31, and the basicity increasing to 2.38 from 1.74. These new parameters predict for the whole 37 point data set a slight increase in absolute error to 26.3% with no increase in the number or magnitude of outliers.

The solubilities of hexachlorobenzene (T_m = 501.7 K, H_{fus} = 6099.4 cal/mol) in 30 solvents (Fina, Van et al. 2000) for which MOSCED parameters were available were used to regress parameters. The best-fit parameters result in a 26% AAD with a comparison of experimental and predicted values in Figure 2-5. The large dispersion term is a result of the number of free electrons from the benzene ring and attached chlorine atoms. The non-zero polarity parameter is consistent with that of other single

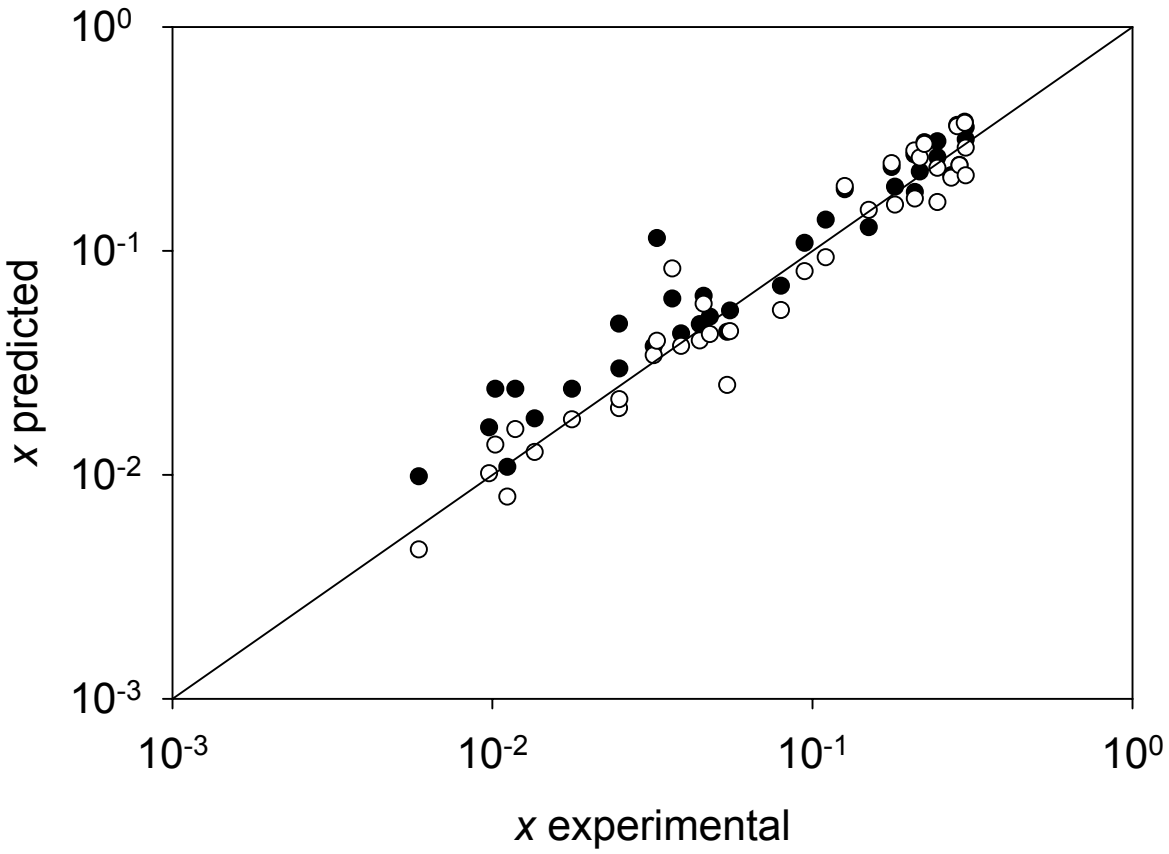

Figure 2-4. Predictions of the mole fraction solubility of phenanthrene with UNIFAC(●) and MOSCED(○).

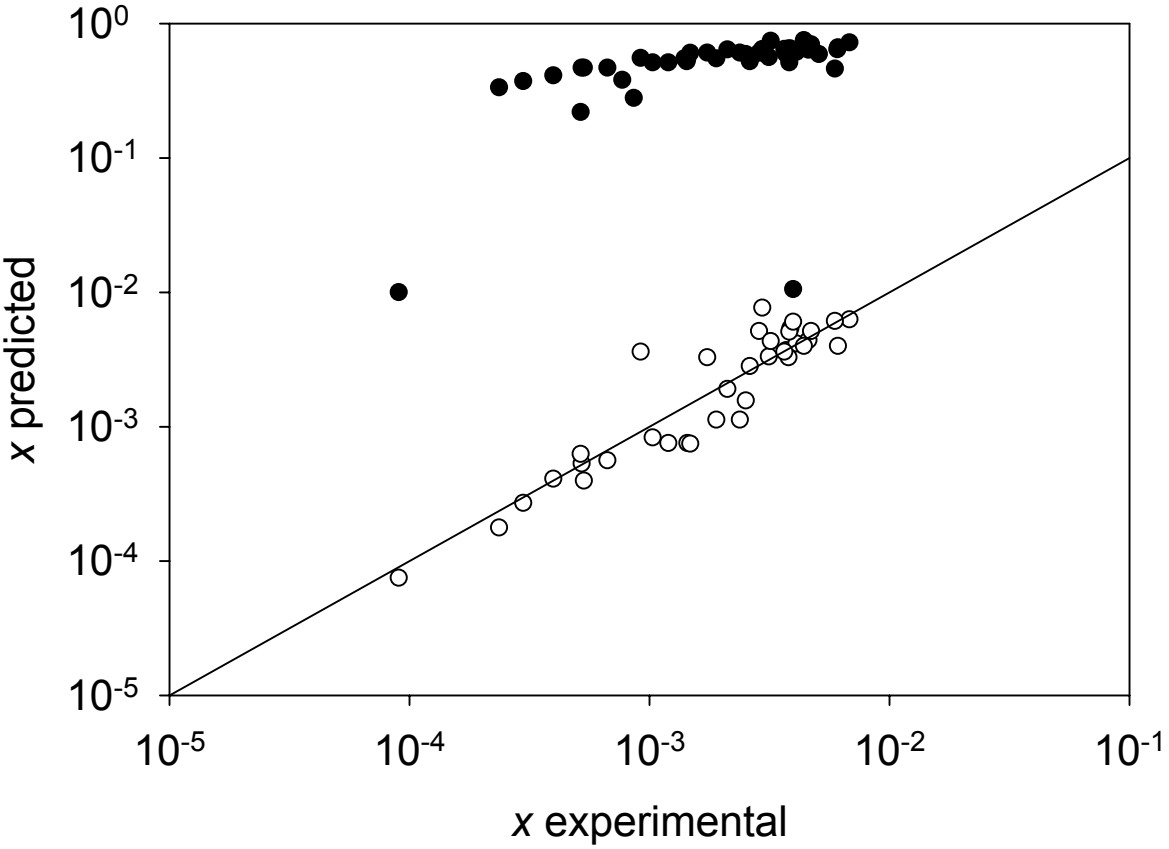

Figure 2-5. Predictions of the mole fraction solubility of hexachlorobenzene with UNIFAC(●) and MOSCED(○).

ring aromatic solvents (benzene $\tau = 3.95$, toluene $\tau = 3.22$). There are no acidic moieties in the compound thus $\alpha = 0$ and the electron withdrawing chlorines have eliminated the basicity of the aromatic ring. The results for the UNIFAC model show a complete failure at predicting the solubility, with the possible exception of the solubility in 1,4-dioxane and less so in methanol. This may be because the UNIFAC model does not account for any neighboring group effects and treats the six chlorine substituents as the sum of six single chlorine substituents.

The capability of MOSCED to correlate a multifunctional molecule was tested with acetaminophen with solubility data for 19 solvents (Granberg and Rasmuson 1999). The large hydrogen bond donor value is expected because of the two acid protons in the molecule and the hydrogen bond acceptor value is reasonable because of the carbonyl and aromatic ring moieties. The smaller polarity term may be due to the para positioning of the two side groups off the ring thus a small net dipole in solution. The MOSCED model is able to correlate the solubility data over 4 orders of magnitude in solubility with the results shown in Figure 2-3. The solubility data in the chlorinated methane solvents are available in the literature but were not used in the correlation because they were only measured once and were not intuitively consistent, but they are included in Figure 2-3. A comparison of the solubility prediction with the UNIFAC model is not possible because the molecule cannot be accurately constructed with the available groups due to a missing secondary amine attached to an aromatic carbon group. Rasmuson (Gracin, Brinck et al. 2002) has suggested two approximations for building acetaminophen from the available

UNIFAC groups, although both approximations resulted in several very large deviations from experimental values.

The solubilities of p-nitroaniline and N,N-dimethyl-p-nitroaniline were also considered. The difference in shift in the UV of this pair of probe compounds in liquid solvents is the basis for the basicity parameter of the Kamlet-Taft scale. The scale is based upon the assumption that the only differences in interaction in solution are due to the change in the amine group from the acidic primary amine to the non-acidic tertiary amine. The solubilities of p-nitroaniline in 39 solvents and N,N-dimethyl-p-nitroaniline in 33 solvents were used to regress the solute parameters (Huyskens, Morissen et al. 1998). The results of the fit are shown in Figure 2-4. We can see from the regressed MOSCED parameters, as shown in Table 2-3, the dispersion and polarity terms are similar for the two compounds, and the difference in hydrogen bond acidity is expected, with a large term for p-nitroaniline (α = 11.14) and zero for the dimethyl compound. We do see some more significant differences in the parameters for the hydrogen bond basicity term, which could be due to some differences in stability of the possible resonance structures of the two compounds. The UNIFAC model does have an aromatic amine group available, but it is missing many of the interaction parameters for the solvents in this data set and for those available it generally under predicts the solubility. There is no aromatic tertiary amine group available in the UNIFAC model and thus no predictions can be made for N,N-dimethyl-p-nitroaniline.

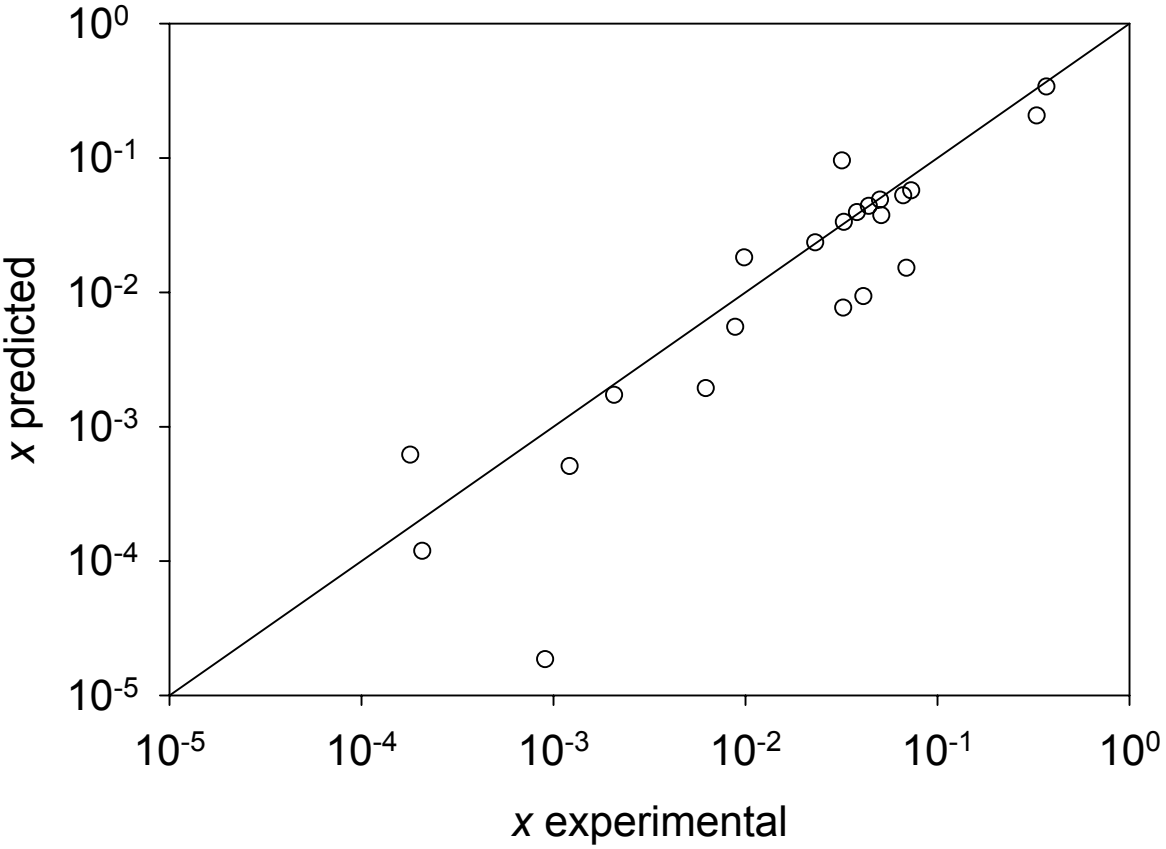

Figure 2-6. Predictions of the mole fraction solubility of acetaminophen with UNIFAC(●) and MOSCED(○).

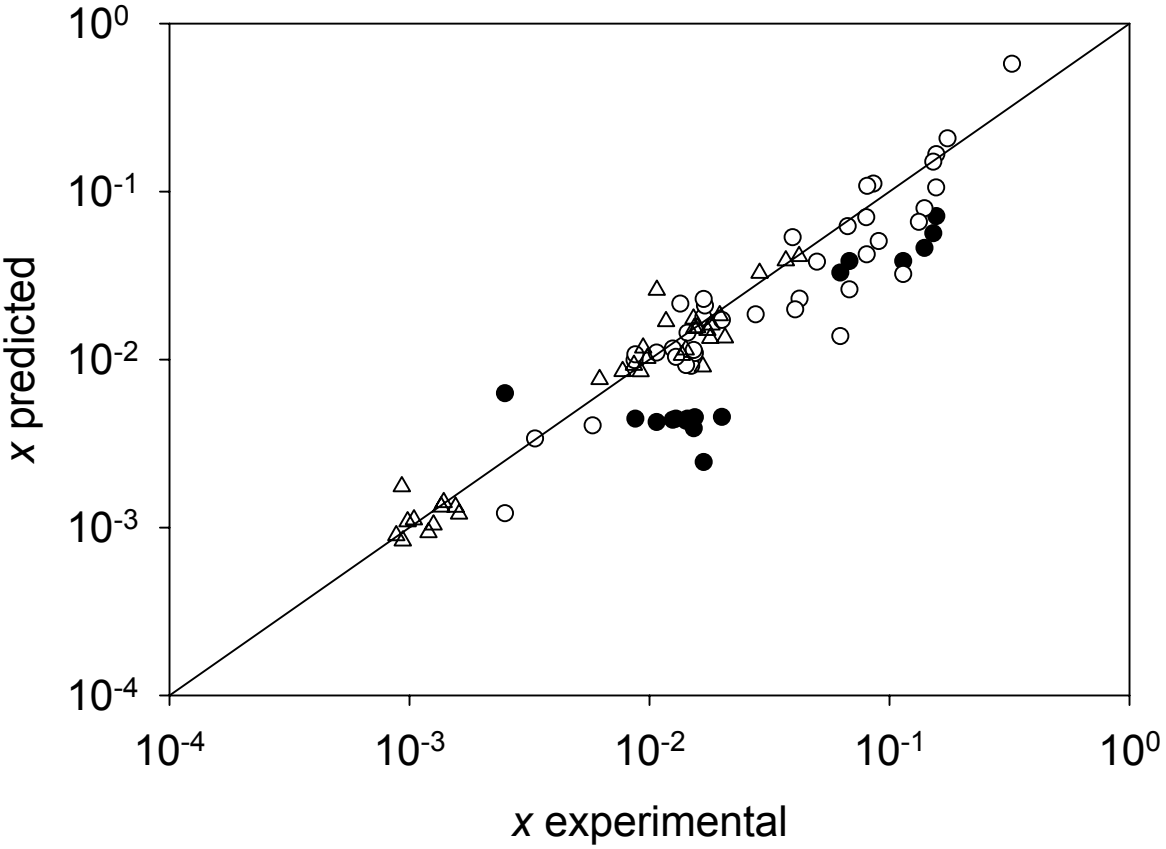

Figure 2-7. Predictions of the mole fraction solubility of p-nitroaniline with UNIFAC(●) and MOSCED(○) and N,N-dimethyl-p-nitroaniline with MOSCED (△).

Table 2-4. Pure component parameters and regressed MOSCED parameters for solid solutes. AAD% and number of data points (n) for both UNIFAC and MOSCED predictions.

Solute	v	λ	τ	q	α	β	UNIFAC AAD% (n)	MOSCED AAD% (n)	Ref.
2-hydroxybenzoic acid	119.6	14.72	4.77	0.90	22.49	4.89	47.1% (14)	20.1% (14)	[14]
2-nitro-5-methylphenol	123.5	17.10	7.76	0.90	1.04	2.53	---	19.7% (17)	[5]
4-nitro-5-methylphenol	123.5	17.60	7.06	0.90	25.94	4.39	---	37.4% (19)	[7]
acenaphthene	137.8	18.26	4.31	0.90	0.00	1.24	27.0% (36)	14.8% (27)	[16]
acetaminophen	105.4	18.45	2.67	0.90	16.19	13.18	---	36.6% (19)	[27]
anthracene	183.3	18.02	4.73	0.90	0.00	1.29	24.0% (43)	24.8% (36)	[35]
benzil	183.0	18.90	6.25	0.90	1.74	3.61	78.8% (36)	13.3% (28)	[21]
biphenyl	149.4	17.28	5.09	0.90	0.00	0.43	12.4% (42)	13.2% (32)	[17]
diphenyl sulfone	161.5	16.75	9.74	0.90	0.00	7.45	---	22.3% (32)	[19]
diuron	164.8	16.99	4.12	0.90	7.88	9.88	---	36.3% (37)	[15]
fluoranthene	184.4	19.96	4.59	0.90	2.51	2.10	54.6% (45)	28.0% (32)	[35]
hexachlorobenzene	164.9	19.64	2.13	0.90	0.00	0.00		26.3% (30)	[18]
ibuprofen	214.2	15.20	5.02	0.90	10.11	3.54	22.2% (38)	20.6% (38)	[26]
monuron	152.8	16.44	5.48	0.90	7.16	9.65	---	22.0% (32)	[13]
naphthalene	131.0	17.78	4.53	0.90	0.00	3.03	11.0% (36)	10.9% (33)	[2]
p-aminophenylacetic acid	137.9	16.08	7.23	0.90	5.74	7.41	---	38.6% (25)	[26]
phenanthrene	167.1	18.48	5.31	0.90	0.00	1.74	36.7% (37)	23.8% (37)	[2]
phenylacetic acid	110.9	14.29	1.95	0.90	15.16	3.57	29.4% (9)	11.8% (9)	[26]
p-hydroxybenzoic acid	95.7	15.16	3.68	0.90	31.27	4.98	39.5% (9)	20.4% (9)	[26]
p-hydroxyphenylacetic acid	123.9	14.45	4.18	0.90	17.40	5.62	48.6% (30)	50.1% (32)	[26]
p-nitroaniline	131.6	18.15	8.94	0.90	11.14	6.70	69.4% (17)	31.3% (39)	[38]
N,N-dimethyl-p-nitroaniline	140.8	18.02	8.25	0.90	0.00	4.20	---	20.6% (33)	[38]
pyrene	184.9	18.63	5.81	0.90	0.00	2.45	39.9% (30)	35.8% (27)	[35]
thianthrene	156.0	19.54	5.14	0.90	0.00	2.71	---	16.5% (18)	[20]
trans-stilbene	188.6	17.98	4.79	0.90	0.00	3.24	41.6% (16)	19.9% (16)	[1]
xanthene	150.0	19.07	4.84	0.90	0.00	1.52	---	18.6% (27)	[45]

The MOSCED model is readily extended to predict solid solubility in mixed solvents. Because the model predicts only the infinite dilution activity coefficients, the accurate prediction of solubility in mixed solvents is strongly dependent upon the ability of the activity coefficient model to predict the binary solvent behavior. There is often a solvent pair that will give a maximum in solubility. One example of a synergistic effect of a solvent mixture is the solubility of 2-nitro-5-methylphenol in a hexane/ethanol mixture (Buchowski, Domanska et al. 1979). The prediction of the MOSCED model with the Wilson g^E model is in good agreement with the experimental data as shown in Figure 2-8. One explanation for the existence of this maximum in solubility is the hexane interfering with the hydrogen bond network of the ethanol solvent sufficiently to allow some solvation of the 2-nitro-5-methylphenol compound that possess both acidic and basic moieties.

Another system that exhibits a maximum in solubility with a mixed solvent is the solubility of acetaminophen in a 1,4-dioxane + water mixture as measured by Bustamante (Bustamante, Romero et al. 1998). At a 50/50 mole ratio of solvent, acetaminophen has a solubility over four times greater than the solubility in pure 1,4-dioxane. This maximum at equal mole fraction implies a specific interaction of both solvents with the solute molecule. The acidic and basic moieties on the acetaminophen molecule are solvated by the basic ether and the acidic protons of the water molecule. As shown in Figure 2-9, the MOSCED model with the UNIQUAC g^E model is able to predict the maximum in solubility at around a 50/50 mixture, however the magnitude of the maximum is under-predicted. Considering the challenge of predicting aqueous

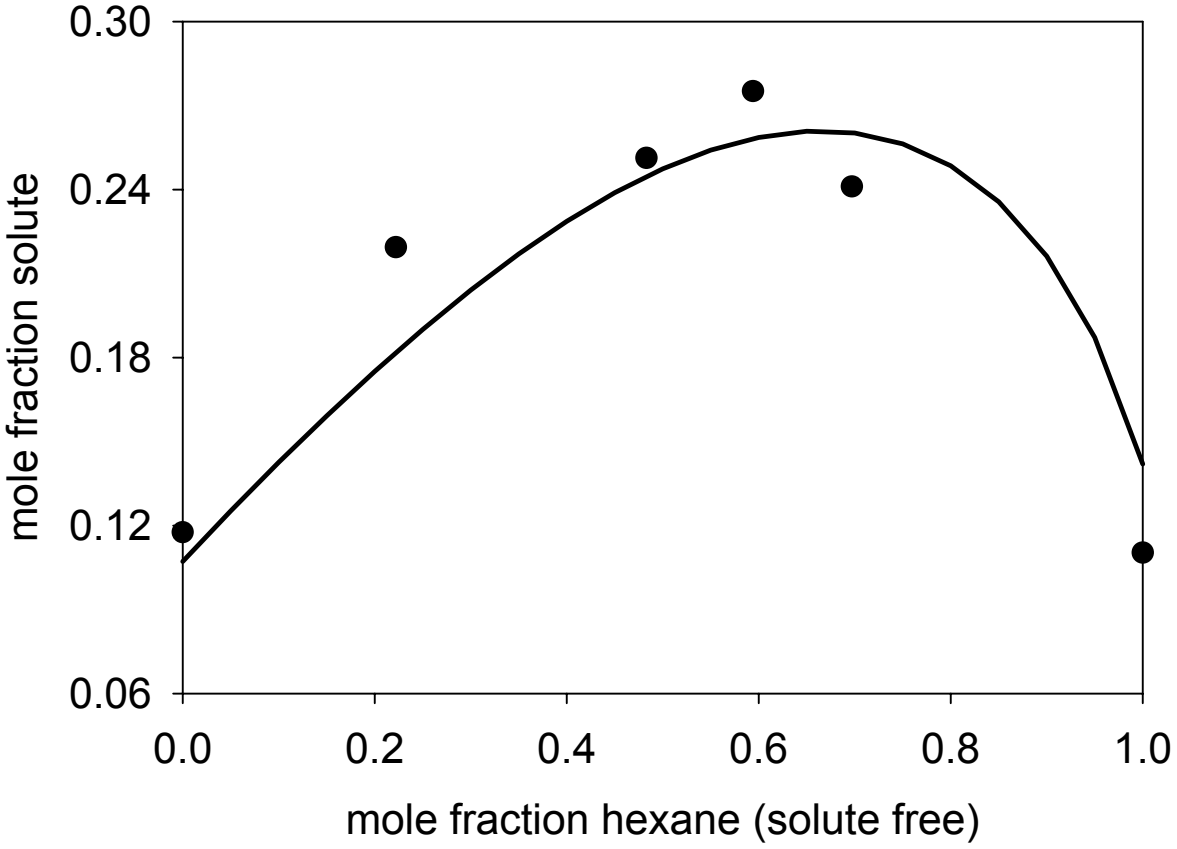

Figure 2-8. Mole fraction solubility of 2-nitro-5-methylphenol (●) in hexane + ethanol mixtures at 298 K (Buchowski, Domanska et al. 1979). Solid line MOSCED with Wilson.

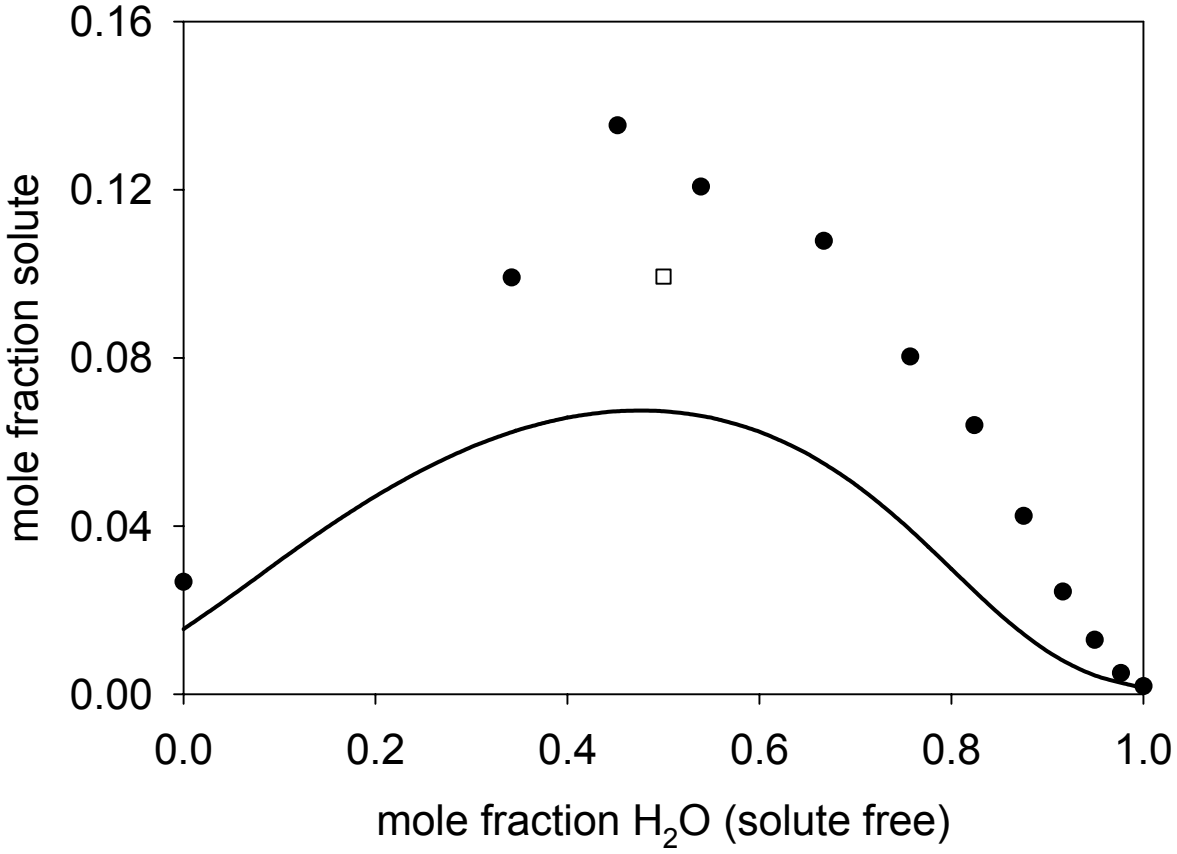

Figure 2-9. Mole fraction solubility of acetaminophen in dioxane + water mixtures at 298.15 K. (●) Bustamante,et al., (□) this work. Solid line MOSCED with UNIQUAC.

systems for many thermodynamic models, this result is promising.

Extension of Model to Gas Solubility

The MOSCED model like regular solution theory is suitable for prediction of gas solubility. To correlate MOSCED parameters for gaseous solutes, the hypothetical liquid molar volume and the hypothetical liquid fugacity are needed at a reference temperature. Prausnitz and Shair (Prausnitz and Shair 1961) correlated the molar volume, fugacity, and solubility parameter using regular solution theory to predict gas solubility. Because these three necessary parameters are not independent of each other the hypothetical liquid fugacity was set to the existing regular solution theory values and only the molar volume and MOSCED model parameters were adjusted to correlate solubility data. It was found that only the dispersion parameter was necessary to accurately correlate solubility data for oxygen, argon, nitrogen, and carbon monoxide. However for carbon dioxide, the polarity and acidity parameters along with the dispersion parameter were necessary for accurate correlation.

Experimental Henry's constant data at 1.103 bar and 298.15 K for oxygen, argon, nitrogen, carbon monoxide, and carbon dioxide were taken from the IUPAC Solubility Series. The optimum values of the molar volume and parameters are shown in Table 2-5 and the experimental values versus the predicted values are shown in Figure 2-6 for the gases with lower critical temperatures, and in Figure 2-7 for carbon dioxide. The parameters for argon, oxygen, nitrogen, and carbon monoxide differ from the regular solution theory values because of the addition of a Flory-Huggins contribution with the

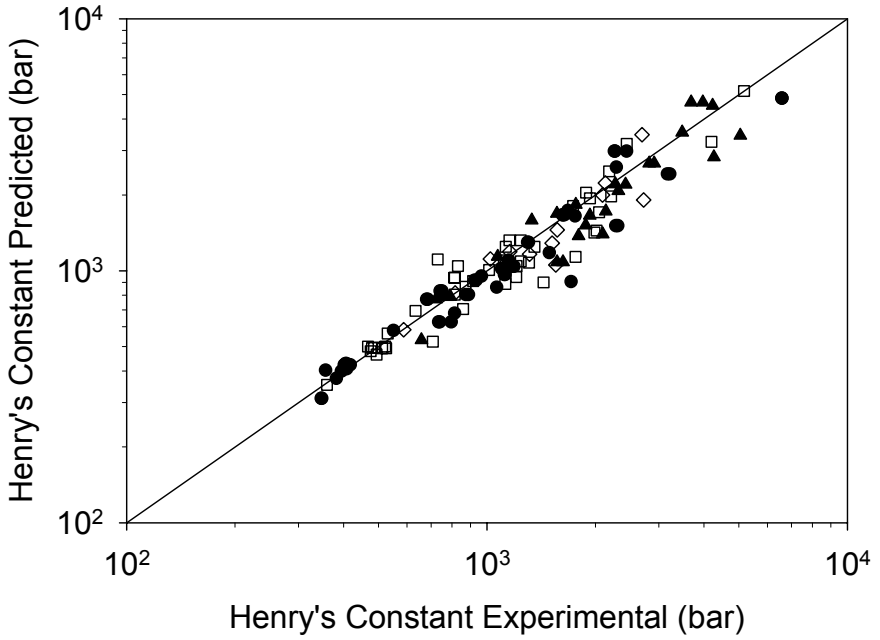

Figure 2-10. MOSCED prediction versus experimental Henry's constants for Argon(●), Oxygen(□), Nitrogen(▲), and Carbon Monoxide(◇)

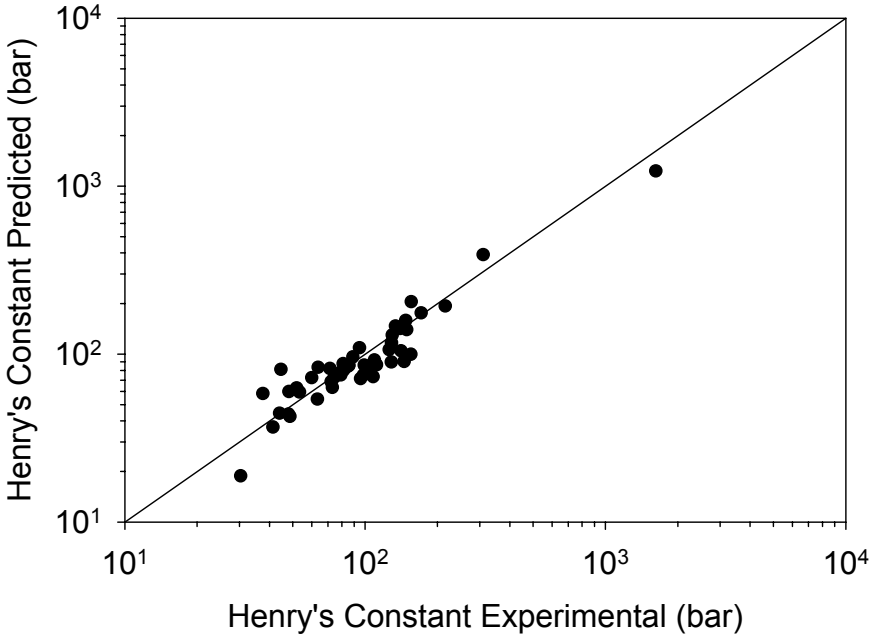

Figure 2-11. MOSCED prediction versus experimental Henry's constants for Carbon Dioxide (●).

Table 2-5. MOSCED parameters for gaseous solutes at 298.15 K and AAD% of the prediction.

Solute	f^L(bar)	v^L (cm^3/mol)	λ	τ	q	α	β	AAE %
Argon	300	57.1	9.84	0	1.0	0	0	11.8 %
Oxygen	300	52.9	8.84	0	1.0	0	0	13.0 %
Nitrogen	350	50.0	7.48	0	1.0	0	0	15.5 %
Carbon Monoxide	325	49.0	8.15	0	1.0	0	0	12.2 %
Carbon Dioxide	37.3	42.2	8.72	5.68	1.0	1.87	0	16.8 %

MOSCED model.

The optimum MOSCED parameters for carbon dioxide reveal some interesting aspects about the behavior of CO_2 in solution. CO_2 has no net dipole moment, it does have a quadrupole moment, and the non-zero polarity is necessary to explain the higher than expected solubility in polar solvents. The high solubility of CO_2 in basic solvents can be explained by the Lewis acidity in solution of carbon dioxide. This acidity is accounted for in the small but significant α parameter allowing for accurate prediction of solubility.

Summary

The MOSCED model has been expanded to measured infinite dilution activity coefficient data measured since the original formulation. Parameters for 130 solvents were fit to 6441 data points to an average error of 10.6%. The MOSCED model is intuitively appealing and has the quantitative capabilities to aid in solvent selection for chemical processes. Because MOSCED only predicts the infinite dilution activity coefficients, any suitable activity coefficient model can be used to extrapolate to finite compositions. The model offers a useful companion to existing models like the UNIFAC model for prediction of phase equilibria.

The MOSCED model has been successfully applied to the prediction of solid solubility. For 26 solutes of various functionalities the solubility was predicted with an average error of 24.9%. Only limited solubility data in a chemically diverse solvent set is necessary to correlate descriptive parameters for a given solute and then solubility can be

predicted for other solvents with MOSCED parameters. From the predicted infinite dilution activity coefficients, the Wilson activity coefficient model was able to predict successfully solubility in mixed solvents. Also, the model was extended to include gaseous solutes and was able to successfully correlate solubility for several gases including carbon dioxide.

Nomenclature

aa = MOSCED Flory-Huggins exponent
ΔC_p = equation of state volume parameter
c = cohesive energy density
d_{12} = MOSCED Flory-Huggins type contribution
ΔH_{vap} = enthalpy of vaporization
ΔH_{fus} = enthalpy of fusion
POL = MOSCED dipolarity asymmetry
q = MOSCED induction parameter
R = universal gas constant
T = temperature
v = molar volume

Greek

α = MOSCED hydrogen bond acidity parameter
β = MOSCED hydrogen bond basicity parameter
δ = solubility parameter
γ = activity coefficient
λ = MOSCED dispersion/polarizability parameter
τ = MOSCED dipolarity parameter
ψ = MOSCED dipolarity asymmetry parameter
ξ = MOSCED hydrogen bonding asymmetry parameter

Superscripts and Subscripts

fus = of fusion
m = at the melting point
s = of the solid
T = at the temperature of interest
trans = of transition
vap = of vaporization
1,2 = component indices

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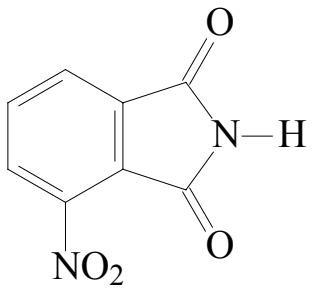
CHAPTER III

EXPERIMENTAL DETERMINATION OF SOLID SOLUBILITY OF MULTI-FUNCTIONAL COMPOUNDS IN PURE AND MIXED NON-ELECTROLYTE SOLVENTS

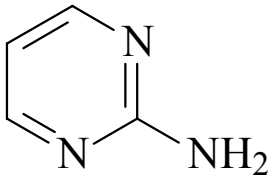
Introduction

The knowledge of solid-liquid equilibria is of clear importance for the design of crystallization processes, including cooling crystallization, evaporative crystallization, and salting-out or anti-solvent crystallization. In Chapter II, the MOSCED model was successfully applied to the prediction of solid solubility in various pure and mixed organic solvents, including aqueous solvent mixtures. In this chapter the model is further applied to the correlation and prediction of newly measured solubilities of some interesting multi-functional solid solutes.

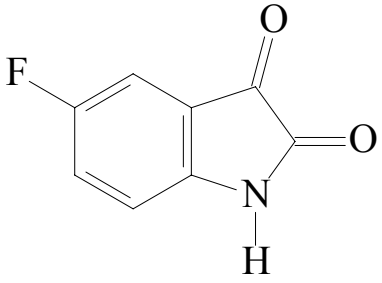
The solid compounds in this study were chosen to demonstrate all types of interactions in solution, i.e. dipolar and hydrogen bonding. In addition, compounds with higher melting points were chosen, so that the ideal solubility is low to simplify the experimental method by eliminating the dilution of the saturated liquid and allow for ease direct sampling by the GC. The four compounds chosen are 3-nitrophthalimide, 5-fluoroisatin, 2-amino-5-nitrobenzophenone, and 2-aminopyrimidine, as shown in Figure 3-1. Given the structure and functionality of the solids, the interactions in solution should



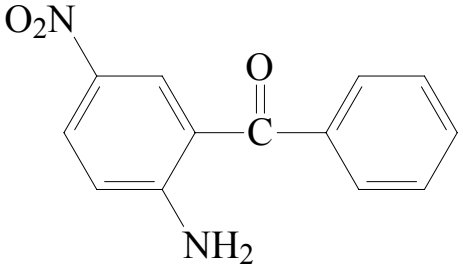
1-A. 3-nitrophthalimide



1-B. 2-aminopyrimidine



1-C. 5-fluoroisatin



1-D. 2-amino-5-nitrobenzophenone

Figure 3-1. Structure of solid compounds studied.

adequately test the MOSCED model.

The organic solvents were chosen to represent a variety of functional groups. The solvents used include the following: cyclohexane, toluene, ethanol, 2-propanol, ethyl acetate, 2-butanone, nitromethane, dioxane, acetonitrile, N,N-dimethylformamide, N-methyl-2-pyrrolidone, chloroform, and dichloromethane. This list of solvents covers many solvent types including polar aprotic, aromatic, and associated compounds and should give a good indication of all the possible solute-solvent interactions. The solubility is also measured in several mixed solvents that have the potential of producing a synergistic effect on the solubility. A mixture of a hydrogen bond donating solvent with a hydrogen bond accepting solvent should increase the solvation of the accepting and donating solutes and cause a maximum in solubility as a function of solvent composition.

The two most prevalent methods for measuring solid-liquid equilibria are the dynamic synthetic method and the static analytical method. In the dynamic synthetic method the solubility is most often determined by adding a known amount of solid to a known amount of solvent, synthesizing the composition, and changing the temperature until the solution goes from a two phase solid-liquid to a single liquid phase. This is similar to the cloud-point determinations often done for liquid-liquid equilibria, where a phase change is visually observed.

In the static analytical method a saturated liquid sample is equilibrated for a given amount of time, after which a sample is carefully withdrawn and analyzed by some physical or chemical analysis. Acree and coworkers have used this technique very often in the measurement of the solubility of polyaromatic solids in organic solvents, using a

ultra-violet detector to measure the solubility (Fina, Sharp et al. 2002). Another analytical technique, commonly referred to as the "dry residue" method (Granberg and Rasmuson 1999), determines the mass of the equilibrium liquid phase and then evaporates the volatile solvent leaving the residual solid matter, which is then also massed. Because of the ability to simultaneously prepare the equilibrium mixtures of the solutes in all the solvents and analyze them with an automatic sampler, in this study the solid-liquid equilibria was determined with a static analytical method using a gas chromatograph with flame ionization detector for composition analysis.

As in Chapter II, the MOSCED model is used to predict infinite dilution activity coefficients of the solid liquid solvent; parameters for the Wilson g^E model are fit to the activity coefficients and the solid-liquid equilibria are predicted for the pure and binary mixed solvents. The possible interactions in solution are discussed given the optimum pure component solute descriptors.

Experimental Materials

The liquid organic solvents were used as received and include: methanol (Aldrich, HPLC, 99.93%), ethanol (Aldrich, anhydrous, 99.5%), 2-propanol (Aldrich, anhydrous, 99.5%), 2-butanone (Aldrich, 99.8+%), ethyl acetate (Fisher, ACS, 99.9%), chloroform (Aldrich, 99.8%), dichloromethane (Riedel-deHaën, 99.8%), acetonitrile (Aldrich, HPLC, 99.93%), nitromethane (Aldrich, HPLC, 98.7%), dioxane (Aldrich, 99+%), N,N-dimethylformamide (Aldrich, anhydrous, 99.8%), N-methyl-2-pyrrolidone (Aldrich, 99%), toluene (Aldrich, anhydrous, 99.8%), cyclohexane (Aldrich, anhydrous, 99.5%),

benzonitrile (Aldrich, HPLC, 99.9%), benzyl alcohol (Aldrich, 98%), chlorobenzene (Aldrich, 99%).

All solid compounds studied were supplied by Aldrich and were used as received: benzil (98%), phenanthrene (98%), anthracene (99%), 2-aminopyrimidine (97%), 2-amino-5-nitrobenzophenone (98+%), 5-fluoroisatin (98%), and 3-nitrophthalimide (97%).

Experimental Apparatus and Procedures

Two methods were used to determine equilibrium solubility of the solids in the organic solvents. The two methods are essentially identical except for how the saturated solution is sampled and whether the sample is diluted prior to analysis. For the first method, equilibrium solutions were prepared in glass vials containing both a solid and liquid phase and placed in a temperature controlled water bath. The saturated solutions were agitated for three to five days to ensure equilibrium condition. A 0.30 ml sample of the saturated liquid phase was removed from the vial using a volumetric pipette accurate to +/- 0.005 ml and the sample mass recorded. The sample was diluted with acetone, up to a 25:1 ratio. . The concentration of the sample was determined using a GC-FID, with a calibration curve for the response prepared over a concentration range. To determined the accuracy of this method, it was compared to the experimental data for the solubility of benzil and phenathrenene in several different solvents. Our results are compared to the literature values in Table 3-1. The solubility data of 2-aminopyrimidine was determined by this method.

Table 3-1. Experimental solubility vs. Literature values using the sampling/dilution method for benzil and phenanthrene at 298 K.

Solute	Solvent	x^{exp}	x^{lit}	%AAD	Ref
Benzil	methanol	0.00738	0.00783	-5.7%	Acree
Benzil	2-propanol	0.00837	0.00831	0.7%	Acree
Benzil	ethyl acetate	0.13768	0.14550	-5.4%	Acree
Benzil	toluene	0.13474	0.15040	-10.4%	Acree
Benzil	cyclohexane	0.01107	0.01068	3.7%	Acree
Phenanthrene	methanol	0.00543	0.00589	-7.8%	Acree
Phenanthrene	ethanol	0.01282	0.01114	15.1%	Acree
Phenanthrene	cyclohexane	0.03943	0.03648	8.1%	Acree
Phenanthrene	1-octanol	0.05672	0.05418	4.7%	Acree
Phenanthrene	ethyl acetate	0.13443	0.14990	-10.3%	Acree
Phenanthrene	1,4-dioxane	0.21352	0.21650	-1.4%	Acree

Table 3-2. Experimental solubility vs. Literature values using the direct sampling method for anthracene at 298 K.

Solute	Solvent	x^{exp}	x^{lit}	%AAD	Ref
Anthracene	heptane	0.00122	0.00157	-22%	Acree
Anthracene	cyclohexane	0.00150	0.00157	-5%	Acree
Anthracene	toluene	0.00713	0.00736	-3%	Acree
Anthracene	dioxane	0.00698	0.00838	-17%	Acree
Anthracene	methanol	0.00034	0.00025	35%	Acree
Anthracene	acetone	0.00376	0.00432	-13%	Acree
Anthracene	tetrahydrofuran	0.01384	0.01204	15%	Acree

For sparingly soluble solids a second method was used that varied slightly from the above method. Equilibrium vials were prepared in the same way and placed in vials with a pierceable septum. The sample vials were placed in a temperature controlled sample tray and agitated periodically for three days. The sample tray was attached directly to an automatic sampler on the gas chromatograph and samples were taken directly from the equilibrium vials and injected directly on the GC column and analyzed by FID. To determine the accuracy of this method, the solubility of anthracene was compared to the literature values, and the results are shown in Table 3-2. This method was used to determine the solubility of 2-amino-5-nitrobenzophenone, 5-fluoroisatin, and 3-nitrophthalimide.

The melting point was determined using a Mettler-Toledo melting point apparatus. The enthalpy of fusion at the melting point for all the solids was determined using a DSC at a heating rate of 10°C/min under nitrogen flow.

Experimental Results Pure Solvents

The solubility of 3-nitrophthalimide as a function of temperature is shown in Figure 3-2. The solubility increases with increasing temperature for all compounds except for chloroform. The density of chloroform is greater than that of the solid and therefore the solid phase is suspended in solution causing the potential for sampling errors. However, the solubility data is qualitatively consistent with the data of the similar dichloromethane. 3-Nitrophthalimide is most soluble in the very polar and strongly hydrogen bond accepting compounds of N,N-dimethylformamide and N-methyl-2-

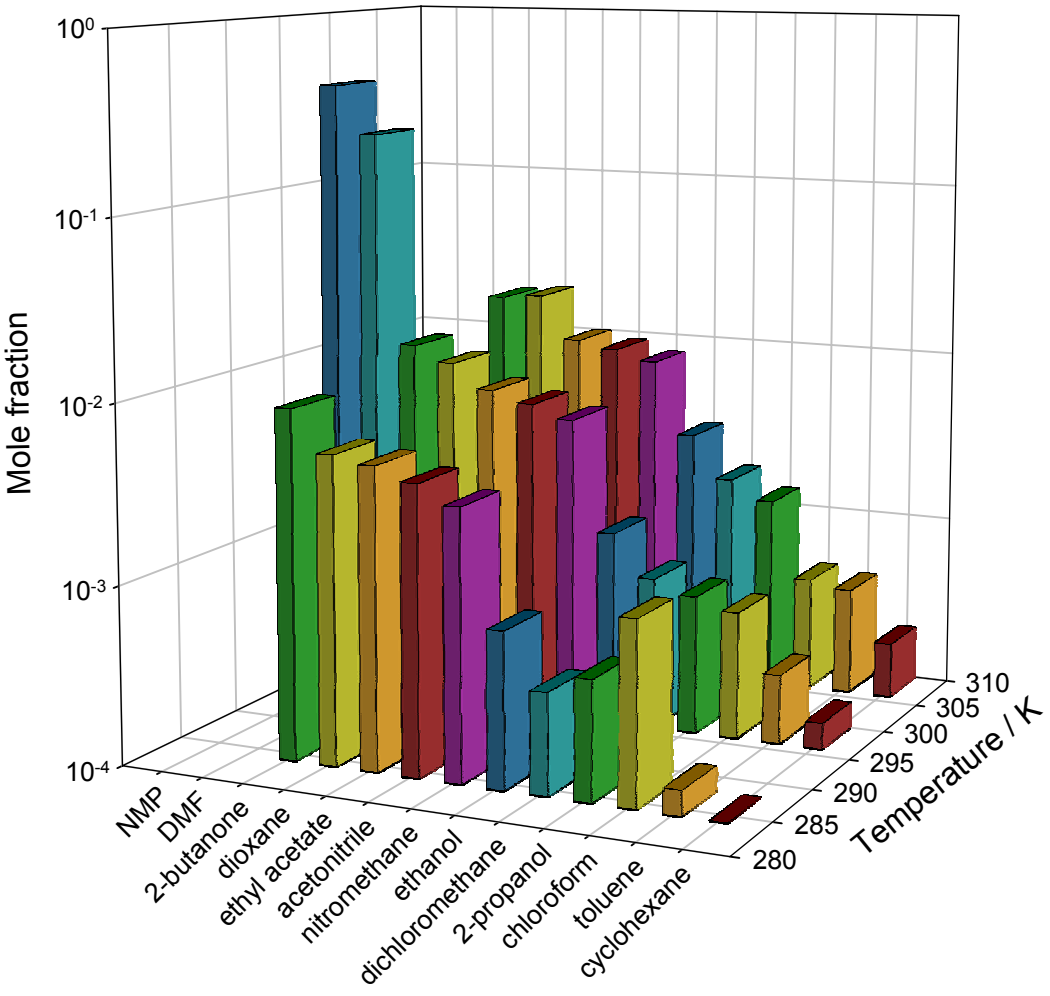


Figure 3-2. Solubility of 3-nitrophthalimide in various organic solvents at 286 K, 298 K, and 308 K.

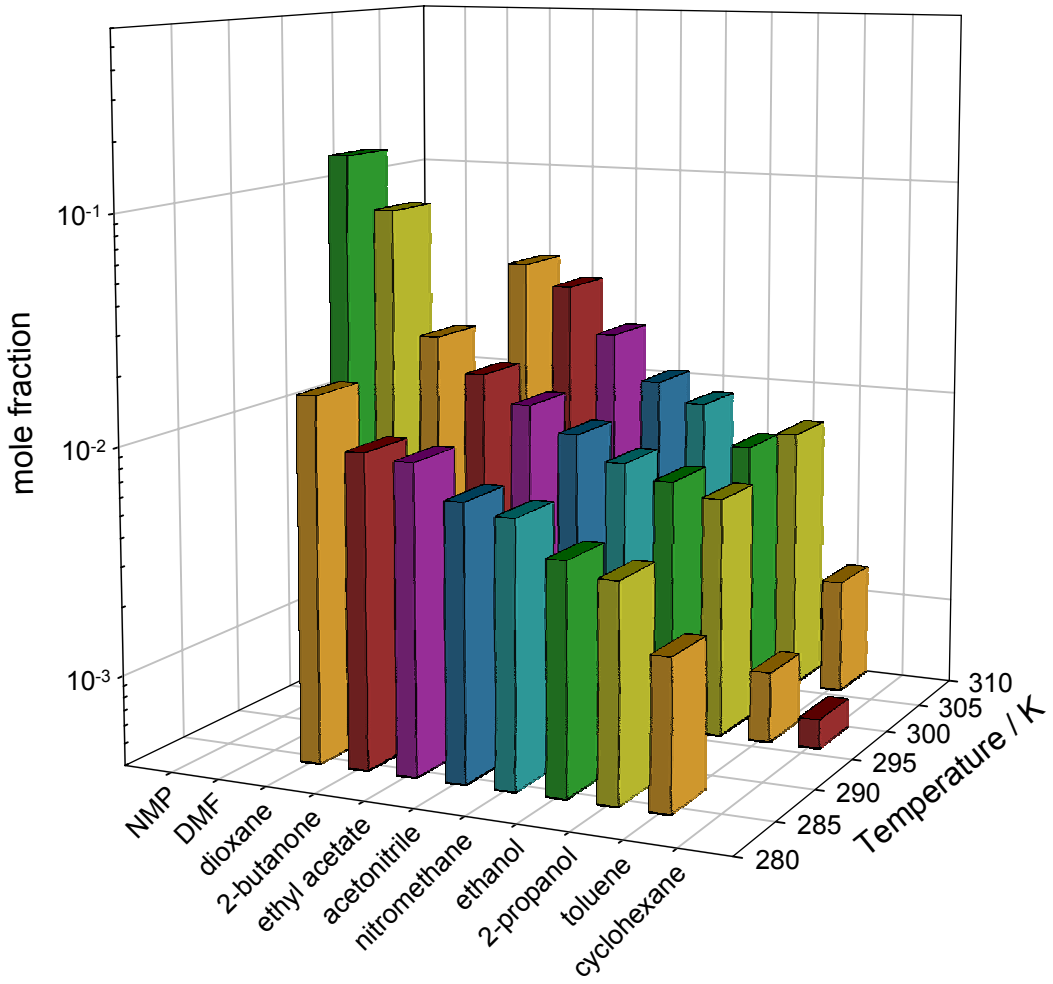


Figure 3-3. Solubility of 5-fluoroisatin in various organic solvents at 286 K, 298 K, and 308 K.

pyrrolidone. For these two solvents the solubility is greater than the ideal demonstrating strong specific interactions, most likely from the acid proton of the 3-nitrophthalimide hydrogen bonding with the basic moieties of the solvents. The solubility is lower in the relatively less basic solvents of 2-butanone, dioxane, ethyl acetate, acetonitrile, and nitromethane. The solubility is lower still in the associated solvents of ethanol and 2-propanol. This indicates that the hydrogen bond association interactions of these solvents are stronger than solute-solvent interactions. In the acidic and essentially non-basic chlorinated solvents, the solubility is also small, indicating a weak hydrogen bond accepting ability of the solute. The solubility is lowest in the non-polar solvents of toluene and cyclohexane, most likely due to the polar nature of 3-nitrophthalimide.

The solubility of 5-fluoroisatin in the range of solvents studied as a function of temperature is shown in Figure 3-3. The solubility trend is very similarly to that of the previously discussed 3-nitrophthalimide. This is not surprising considering the similar structure of the two molecules. The solubility is highest in the strongly basic and polar solvents of N,N-dimethylformamide and N-methyl-2-pyrrolidone, less so in the associated alcohol solvents, and least in the non-polar aromatic and alkane solvents. The characteristics of both 5-fluoroisatin and 3-nitrophthalimide in solution can thus be summarized as polar compounds with a strong hydrogen bond donating ability and a weaker hydrogen bond accepting ability.

The solubility of 2-amino-5-nitrobenzophenone in 14 organic solvents as a function of temperature is shown in Figure 3-4. It can be seen from the figure that the solute is most soluble in the polar and basic solvents of benzonitrile, 2-butanone, and

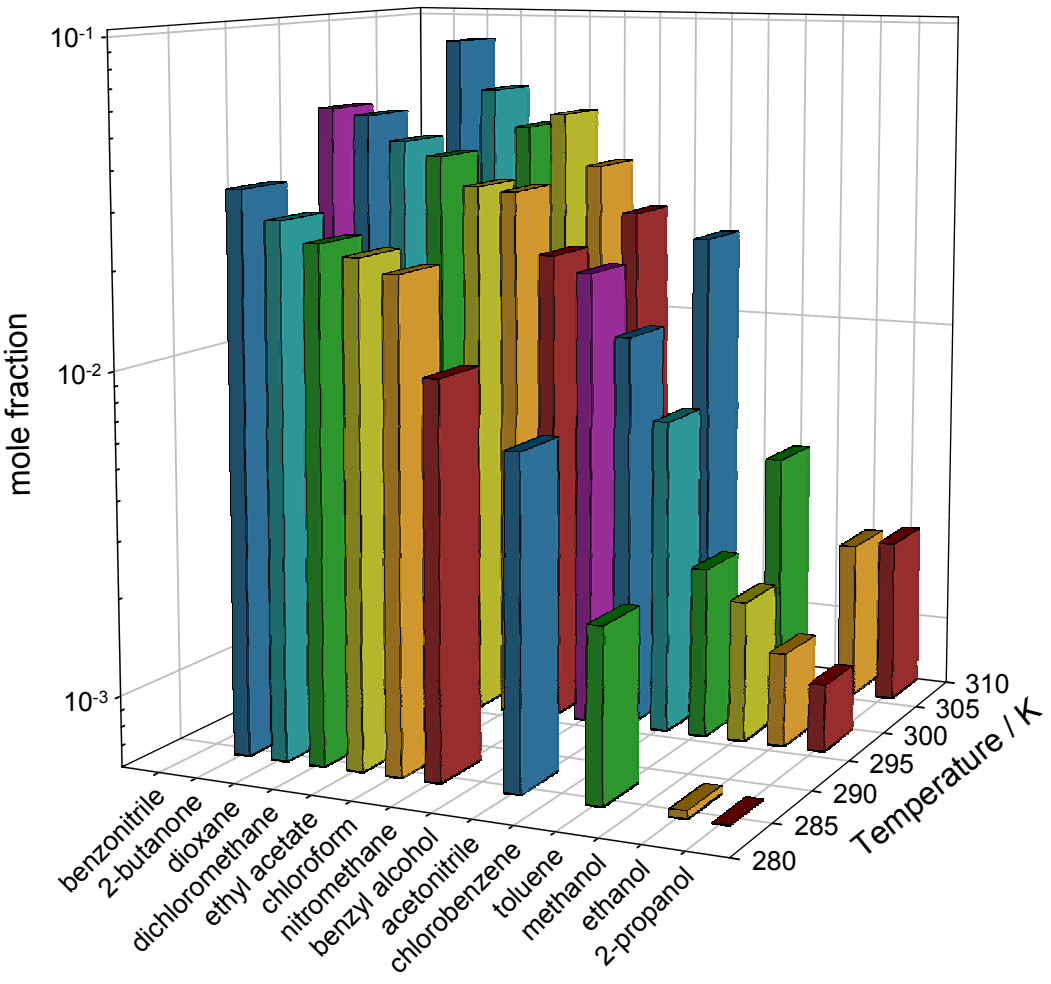


Figure 3-4. Solubility of 2-amino-5-nitrobenzophenone in various organic solvents at 286 K, 298 K, and 308 K.

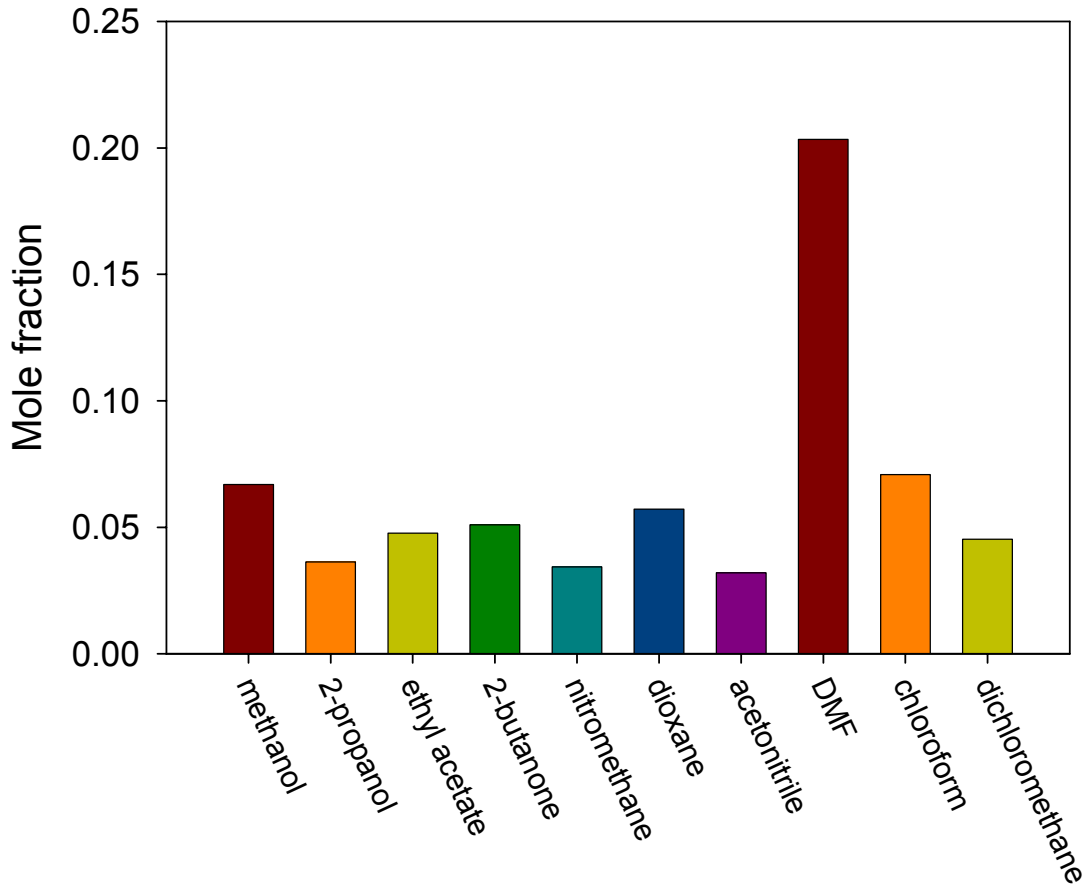


Figure 3-5. Solubility of 2-aminopyrimidine in various organic solvents at 298 K.

dioxane and slightly less but similar solubility in the acidic and non-basic chlorinated solvents dichoromethane and chloroform. This is not surprising since the solute molecule contains both a strong hydrogen donating group (the primary amine) that can associated with the basic solvents and a strong hydrogen bond donating group (the nitro group) that can associate with the acidic solvents. This also indicates that the self association of the solute through hydrogen bonds is not strong enough to prevent solvation by these acidic and basic solvents. The solubility is lowest in the associated alcohol solvents indicating the strength of the hydrogen bond donating and accepting ability of the solute is less than that of the solvent.

The solubility of 2-aminopyrimidine in 10 organic solvents at 298 K is shown in Figure 3-5. The highest solubility by far is in the polar and basic solvent N,N-diemthylformamide. This is probably due to a strong dipolarity of the solute and a strong hydrogen bond donating ability. It is next most soluble in the hydrogen bond donating solvents of methanol and chloroform, indicating a significant hydrogen bond accepting ability of the solute. In the relatively weaker basic and aprotic solvents (when compared to DMF) of dioxane, 2-butanone, and nitromethane, the solubility is slightly less than the hydrogen bond donating solvents. We can conclude the characteristics of 2-aminopyrimdine in solution are strongly dipolar molecule with significant hydrogen bond acidity and basicity with slightly stronger hydrogen bond accepting ability than donating ability. All experimental data is summarized in Appendix G. In the thermodynamic modeling section the intuitive characterization of the solute molecules will be compared to the characteristic descriptors correlated from the MOSCED model.

Experimental Results Mixed Solvents

The solubilities of 3-nitrophthalimide, 5-fluoroisatin, and 2-amino-5-nitrobenzophenone were measured at 298 K in the mixed solvent pairs of ethanol + ethyl acetate and nitromethane + ethanol. For 3-nitrophthalimide there is a maximum in solubility at 0.25 mole fraction of ethanol for both solvent pairs studied, with the maximum being the largest for the nitromethane + ethanol pair at nearly twice the solubility in pure nitromethane. At sufficiently low ethanol concentrations in the mixed solvent, the ethanol will be less self-associated in solution without forming large hydrogen bond complexes and thus will be available to solvate the basic nitro- and carbonyl- groups of the 3-nitrophthalimide compound and result in an increase in solubility over that of the pure ethyl acetate or nitromethane solvent. The solubilities as a function of solvent composition for both solvent pairs are shown in Figures 3-11 and 3-12.

In the case of 5-fluoroisatin both solvent pairs demonstrate very similar behavior, with a maximum in solubility for both solvent pairs at 0.50 mole fraction of the solvent and at nearly twice the solubility of the more soluble pure component. The solubilities as a function of solvent composition for both solvent pairs are shown in Figures 3-13 and 3-14. The hydrogen bond donating ability of ethanol and hydrogen bond accepting ability of the basic solvent also can explain the synergistic effects of the solvent pair. It is not surprising that both compounds, being of similar structure, demonstrate a maximum in solubility for the same solvent pairs. However, the position and magnitude of the maximum as function of solvent concentration is different. This difference may be due to

the degree of self-association possible for the two solutes. While both compounds have similar hydrogen bond donating groups, both possessing secondary amines, 3-nitrophthalimide has a greater number of hydrogen bond accepting moieties with the presence of the nitro- group. In the case of the 3-nitrophthalmide, there is greater competition for forming hydrogen bonds in solution because of the stronger self-association possible with the solute, whereas with 5-fluoroisatin more free solute is available and both basic and acidic solvents can effectively associate with the molecule.

Contrary to the other two solutes, the solubility of 2-amino-5-nitrobenzophenone does not demonstrate a maximum in solubility in either solvent pair. In fact, for both solvent pairs, ethanol behaves as an anti-solvent, where an addition of a small fraction of ethanol decreases the solubility dramatically. This again can be explained considering the potential hydrogen bonds that can form. It is expected that the solid will be self-associated in solution given the hydrogen bonds possible between the primary amine and the nitro- group or carbonyl. In the pure, basic, aprotic solvent, namely ethyl acetate or nitromethane, the solvent is able to effectively associate some of the solid compound. With the addition of small amounts of ethanol, the basic solvent can now also associate with the protic alcohol, thus leaving more solid to self-associate and decreasing the solubility. The solubilities as a function of solvent composition for both solvent pairs are shown in Figures 3-15 and 3-16.

The solubility of 2-aminopyrimidine was measured at 298 K in the mixed solvent pairs of methanol + ethyl acetate, methanol + nitromethane, methanol + acetonitrile, and dioxane + acetonitrile. The solubilities as a function of solvent composition for all

solvent pairs are shown in Figures 3-17 through 3-20. All solvent pairs exhibit a synergistic effect on the solubility. For solvent mixtures of methanol with ethyl acetate, nitromethane, or acetonitrile the solvent composition has a very similar effect on the solubility. As with the other solutes, the combination of hydrogen bond donating and hydrogen bond accepting solvents cause the maximum in solubility observed. For the mixed solvent dioxane with acetonitrile, the maximum in solubility is at lower concentrations of acetonitrile and may be attributed to the smaller molecules of acetonitrile that are able to effectively fill the voids in the solvation shell of 2-aminopyrimidine in pure dioxane.

Thermodynamic Modeling

In Chapter II the MOSCED model was shown to correlate well the solubility of some multifunctional solid compounds in a variety of solvents. In this section, the model is further applied to the investigated solutes in this study. The ideal solubility is calculated in the same manner as in Chapter II (see equation 2-5). The infinite dilution activity coefficients are predicted using the MOSCED model and extend to finite concentration using the Wilson activity coefficient model. The melting point, heat of fusion of the solids, and the regressed MOSCED parameters are shown in Table 3-3.

A comparison of the experimental versus predicted solubility is shown in Figure 3-6 for 3-nitrophthalimide. The model is able to accurately predict the solubility over nearly five orders of magnitude, predicting the greater than ideal solubility ($x_1 > 0.0873$ at 298K) exhibited in the very polar and basic solvents of DMF and NMP and the very low

Table 3-3. MOSCED parameters for solids at 273 K.

Solute	H^{fus} kJ/mol	Tm K	v^L cm^3/mol	λ	τ	q	α	β
2-aminopyrimidine	20.09	400.7	140	18.09	6.52	0.9	6.51	14.5
3-nitrophthalimide	15.57	487.0	140	20.90	9.63	0.9	3.89	8.06
5-fluoroisatin	14.10	498.0	140	20.53	7.12	0.9	4.95	9.52
3-amino-5-nitrobenzophenone	28.50	440.0	150	17.65	8.94	0.9	2.89	6.22

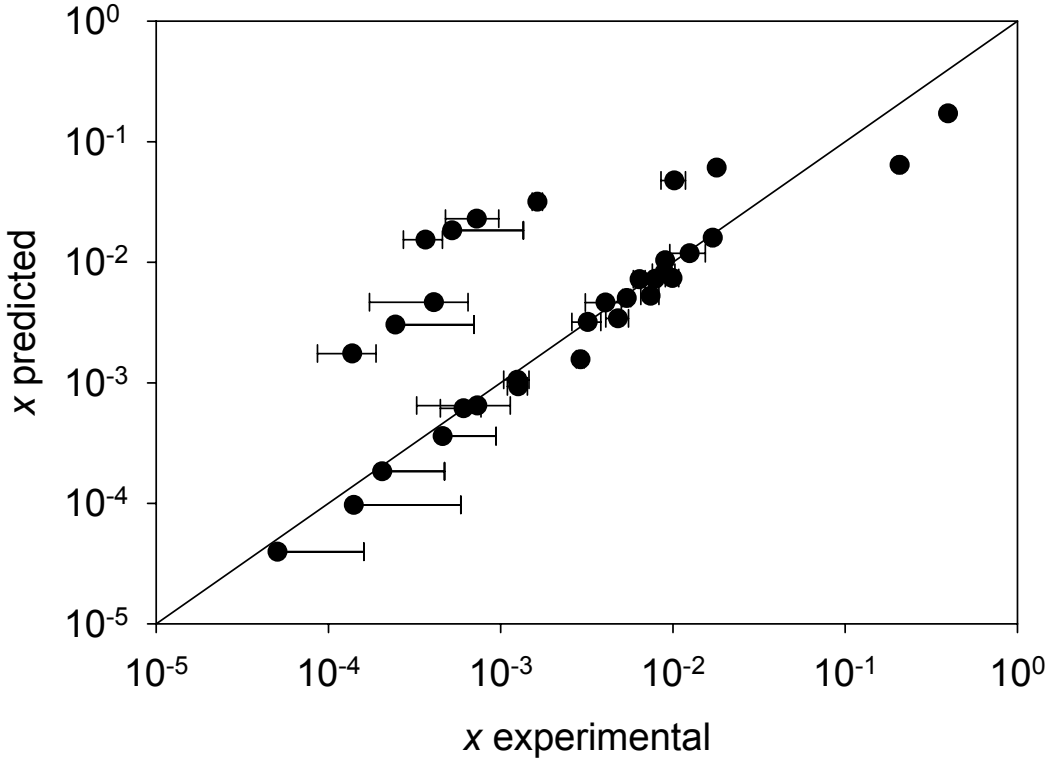


Figure 3-6. Mole fraction solubility of 3-nitrophthalimide in various solvents from 286 to 308 K versus MOSCED predictions.

solubility in cyclohexane. However, the model does over-predict the solubility in toluene, and the chlorinated solvents, chloroform and dichloromethane, which may be a result of an overestimation of the hydrogen bond contribution to the activity coefficient. Additionally the overprediction of the solubility in dioxane may be a result of the inability of the model to account for the different structural conformations of dioxane, i.e. boat or chair, which can greatly affect the magnitude of intermolecular interactions.

The MOSCED model is able to correlate the solubilities of 5-fluoroisatin, as can be seen in Figure 3-7. The model does fail, as in the case of 3-nitrophthalimide, in overpredicting the solubility in toluene. The regressed solute parameters for 3-nitrophthalimide and 5-fluorisatin characterize the two compounds very similarly. Both have a large dispersion term, and a modest dipolarity term similar in magnitude to that of the pyrrolidone solvents, with which it shares some similar structural elements. The 3-nitrophthalimide in fact has a slightly larger dipolarity term which may be due to the position of the nitrous group, whereas the 5-fluoroisatin compound possesses a fluorine side group. The hydrogen bond acidity and basicity terms are also similar in magnitude with the 5-fluoroisatin acidity term being slightly larger, perhaps because the secondary amine is positioned between two carbonyls, where the electro-negative carbonyls would be balanced by a more positive proton. In 3-nitrophthalimide, the secondary amine only neighbors one carbonyl group and would be naturally less protic.

The MOSCED model is able to accurately correlate the solubilities of 2-amino-5-nitrobenzophenone across nearly 4 orders of magnitude, as shown in Figure 3-8. There are no strong outliers to mention, however it does tend to underpredict the solubility

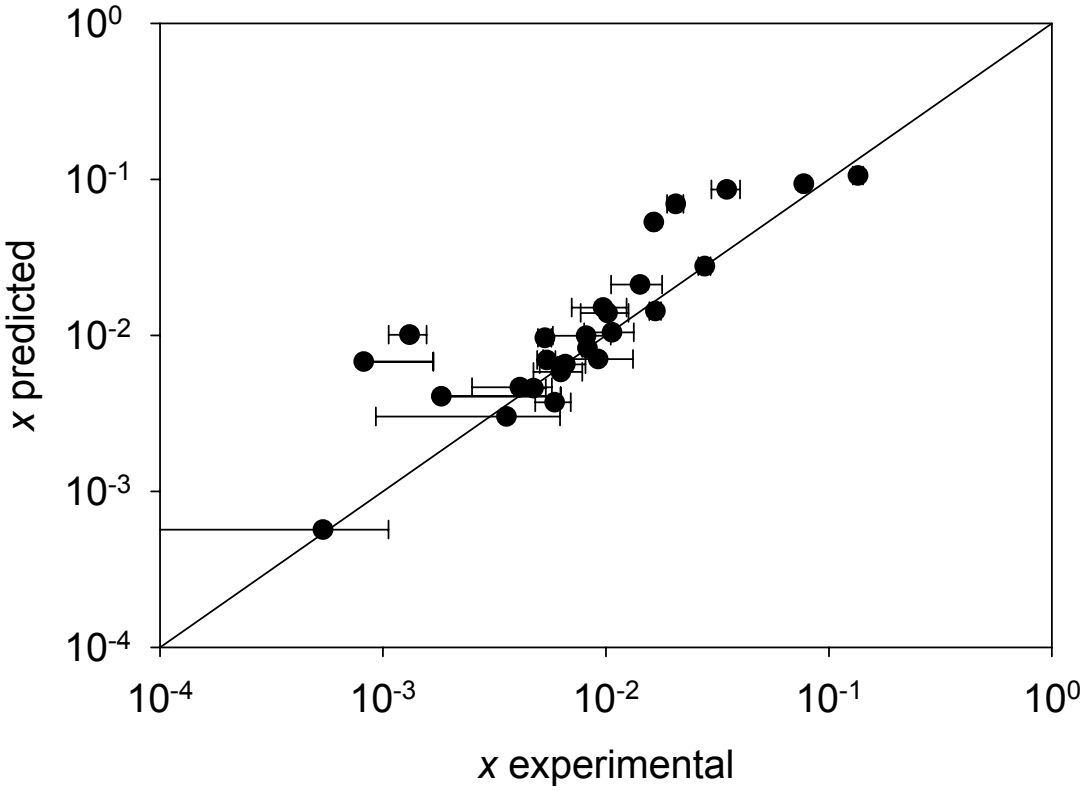


Figure 3-7. Mole fraction solubility of 5-fluoroisatin in various solvents from 286 to 308 K versus MOSCED predictions.

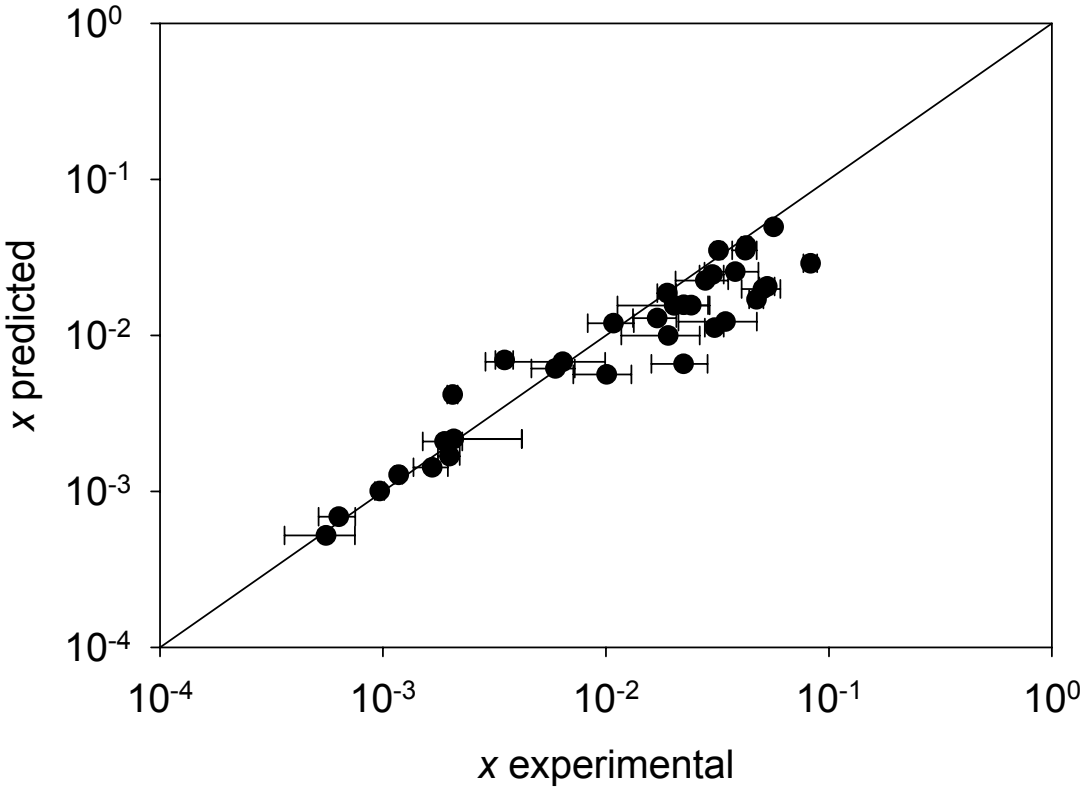


Figure 3-8. Mole fraction solubility of 2-amino-5-nitrobenzophenone in various solvents from 286 to 308 K versus MOSCED predictions.

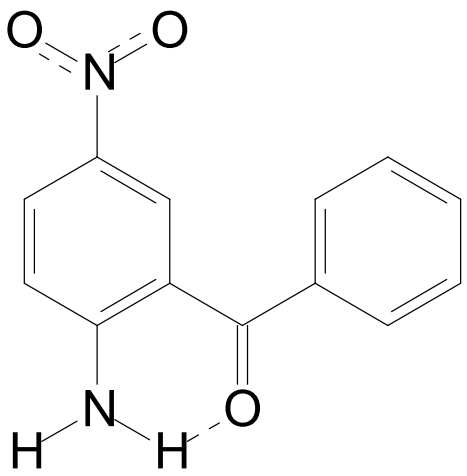


Figure 3-9. Intramolecular hydrogen bonding in 2-amino-5-nitrobenzophenone.

when it does not exactly reproduce the experimental data. The compound descriptors, especially the hydrogen bonding parameters, are smaller than might be expected. Comparing the 2-amino-5-nitrobenzophenone descriptors to those of the similar structured but smaller p-nitroaniline, the dispersion and dipolarity terms are similar, however the acidity term is 2.89, nearly 25% of the value for p-nitroaniline. One possible explanation is the existence of an intramolecular hydrogen bond between the carbonyl and a hydrogen of the secondary amine. The carbonyl is not sterically hindered to rotation and it can easily be in a position to form a hydrogen bond with the neighboring amine, and leaving only one acidic proton available for hydrogen bond donating with the solvent. One possible configuration of the molecule is shown in Figure 3-9. The carbonyl-amine hydrogen bond results in the formation of a six-member ring, thus stabilizing the structure. It may also be possible for both hydrogens to interact with the free electrons on the carbonyl in a 3-dimensional manner, where the protons are orthogonal to the benzene ring plane.

The predictions of the MOSCED model versus the experimental solubilities for 2-aminopyrimidine are shown in Figure 3-10. The model is able to correlate the experimental data very well with the exception of the under-prediction in ethyl acetate. The compound descriptors are consistent with the structure of the molecule, with a large hydrogen bond acidity and basicity term. Because the experimental data only covers one order of magnitude, there are many optimum solutions at values close to each other in the parameter space, thus the error in the parameters are greater.

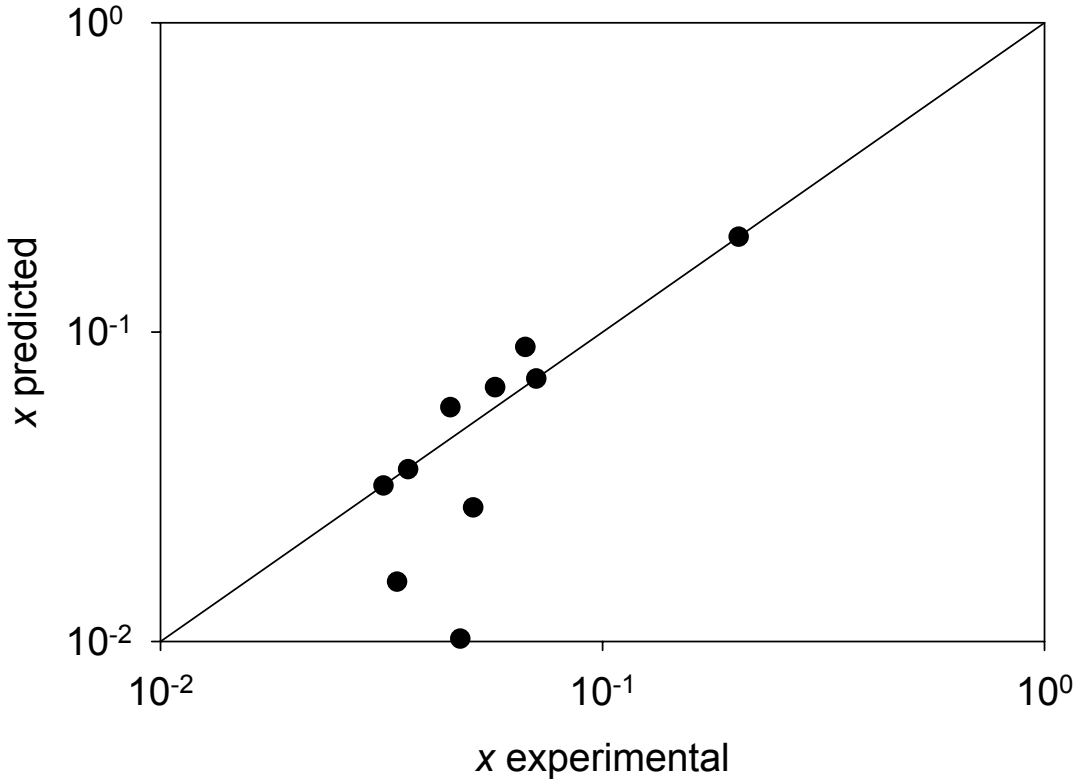


Figure 3-10. Mole fraction solubility of 2-aminopyrimidine in various solvents at 298 K versus MOSCED predictions.

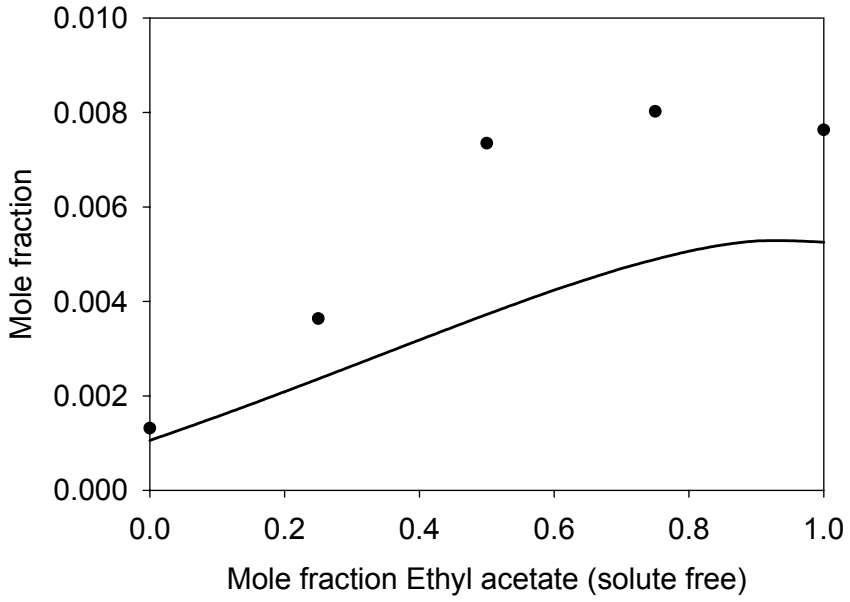


Figure 3-11. Solubility of 3-nitrophthalimide in ethyl acetate/ethanol solvent mixtures at 298K.

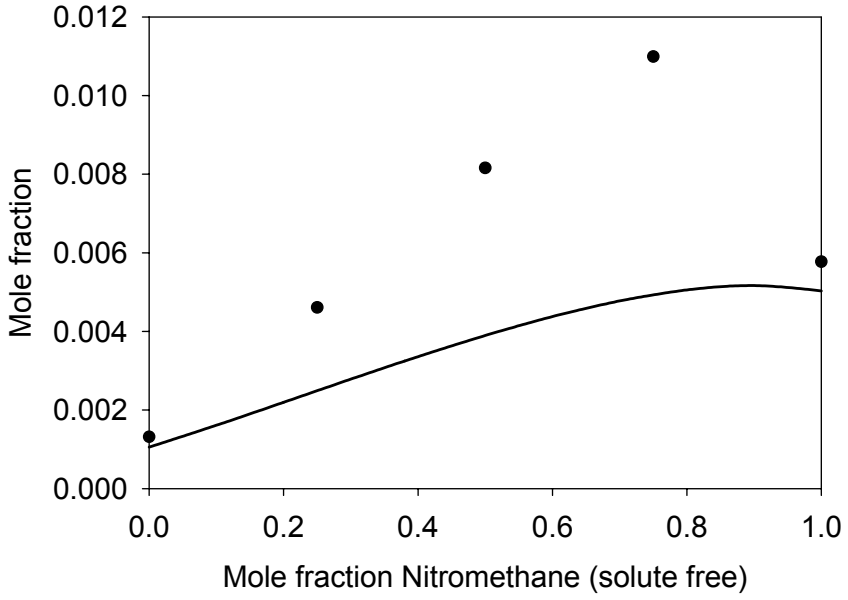


Figure 3-12. Solubility of 3-nitrophthalimide in nitromethane/ethanol solvent mixtures at 298K.

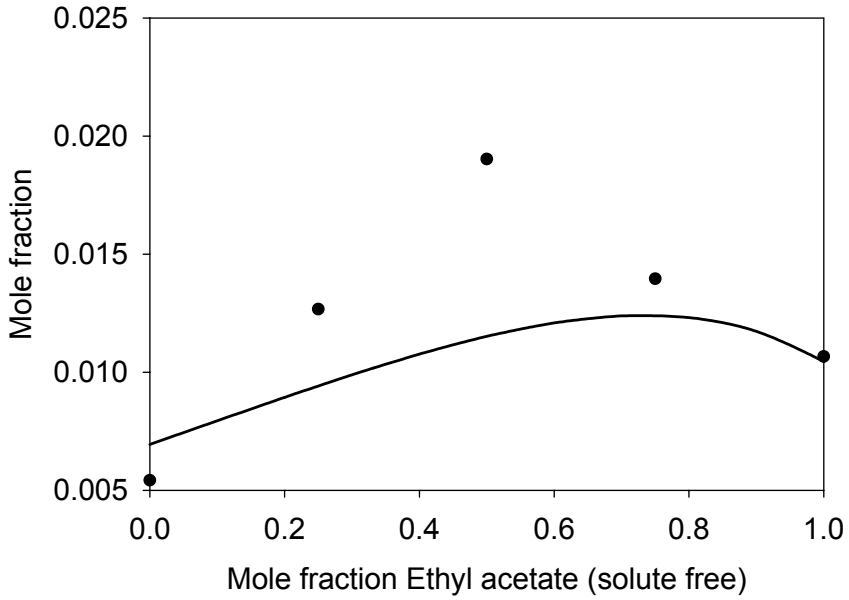


Figure 3-13. Solubility of 5-fluoroisatin in ethyl acetate/ethanol solvent mixtures at 298K.

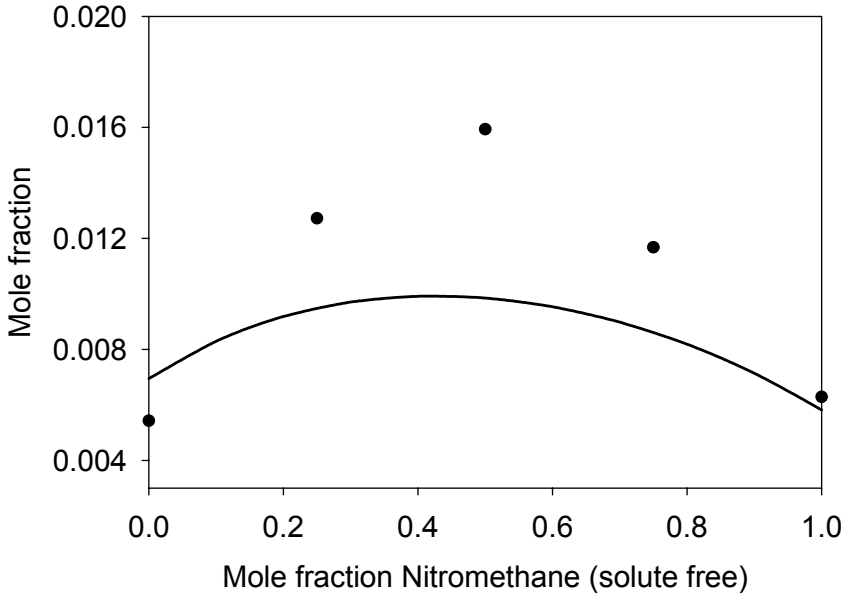


Figure 3-14. Solubility of 5-fluoroisatin in nitromethane/ethanol solvent mixtures at 298K.

For the prediction of the solubility in mixed solvents, in addition to the prediction of the activity coefficient of the solid in the pure solvent, the MOSCED model must predict the mutual activity coefficients of the solvent pair. This makes the predictions more dependent upon the ability of the activity coefficient model to accurately describe the effect of concentration on the activity coefficient away from the infinite dilution region. The results of the predictions for 3-nitrophthalimide and 5-fluorisatin in the mixed solvents are shown in Figures 3-11 through 3-14. For both solid solutes in the two solvent pairs, the model is able to qualitatively predict the existence of a maximum in solubility. In all cases however, the predicted solubility tends to be lower than the experimental values. For the case of 3-nitrophthalimide in ethanol + ethyl acetate (Figure 3-11), the underprediction for the mixture is caused predominantly by the underprediction of the solubility in pure ethyl acetate. The maximum in solubility of 5-fluoroisatin in ethanol + nitromethane is predicted at near the observed solvent concentration, although the model only predicts a solubility roughly 50% of the experimental value.

The predictions for the solubility of 2-amino-5-nitrobenzophenone are shown in Figures 3-15 and 3-16. Although the model underpredicts the solubility of 2-amino-5-nitrobenzophenone in pure nitromethane and ethyl acetate, it does correctly predict the solubility in pure ethanol and reasonably accurately matches the effect that ethyl acetate or nitromethane addition to the solvent mixture has on the solid solubility, at least up to around 20% ethanol concentration.

Of the four solid compounds studied, the best predictions in mixed solvent are for 2-aminopyrimidine, as shown in Figures 3-17 through 3-20. The MOSCED model with

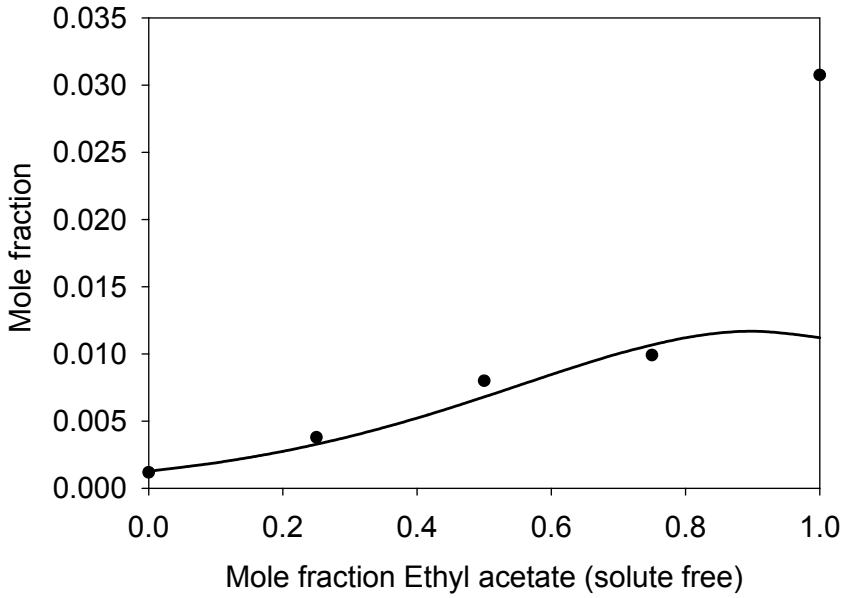


Figure 3-15. Solubility of 2-amino-5-nitrobenzophenone in ethyl acetate/ethanol solvent mixtures at 298K.

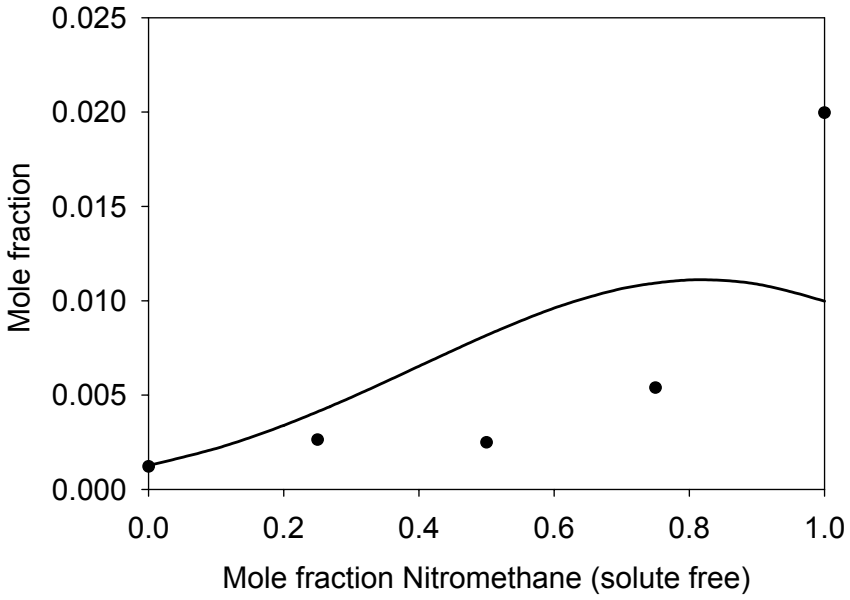


Figure 3-16. Solubility of 2-amino-5-nitrobenzophenone in nitromethane/ethanol solvent mixtures at 298K.

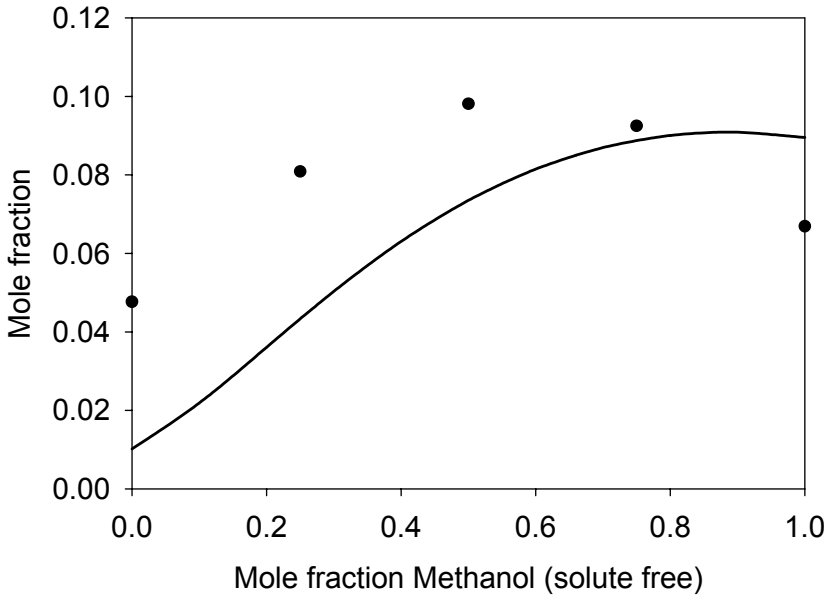


Figure 3-17. Solubility of 2-aminopyrimidine in methanol/ethyl acetate solvent mixtures at 298K.

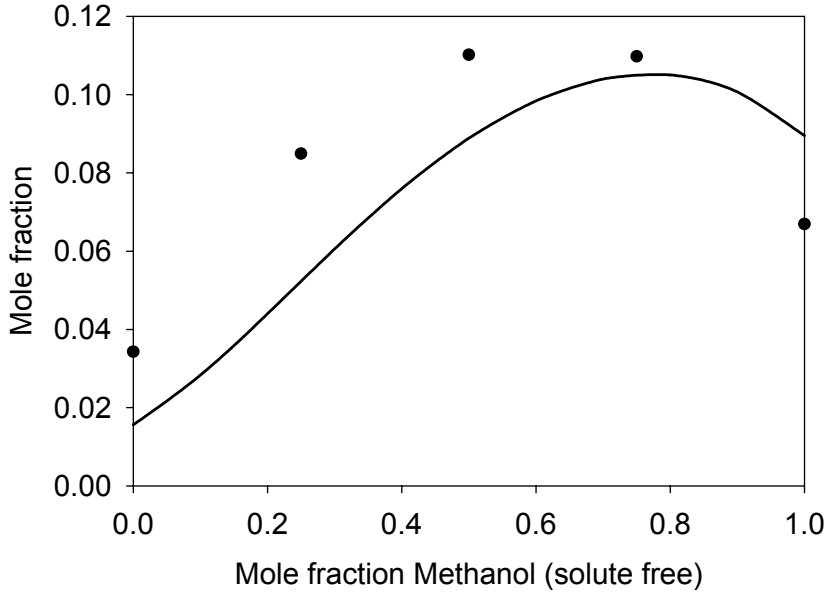


Figure 3-18. Solubility of 2-aminopyrimidine in methanol/nitromethane solvent mixtures at 298K.

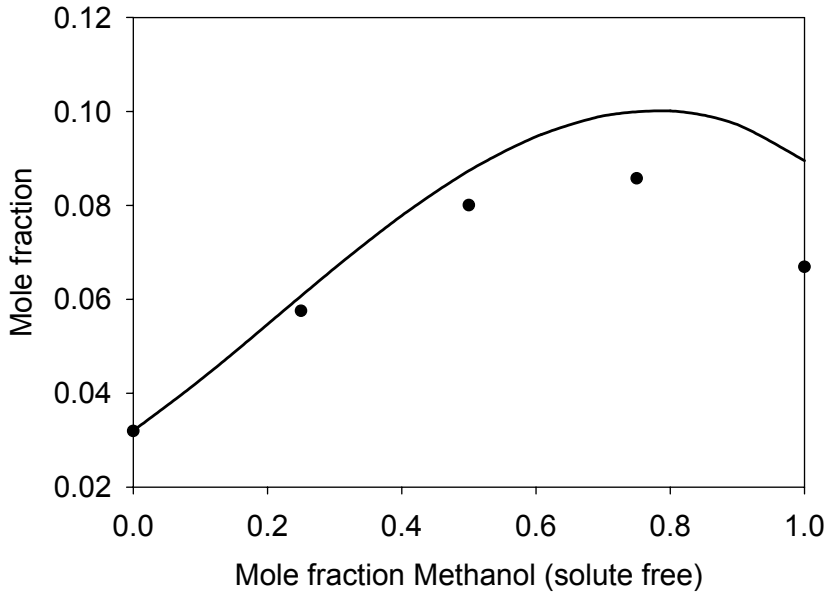


Figure 3-19. Solubility of 2-aminopyrimidine in methanol/acetonitrile solvent mixtures at 298K.

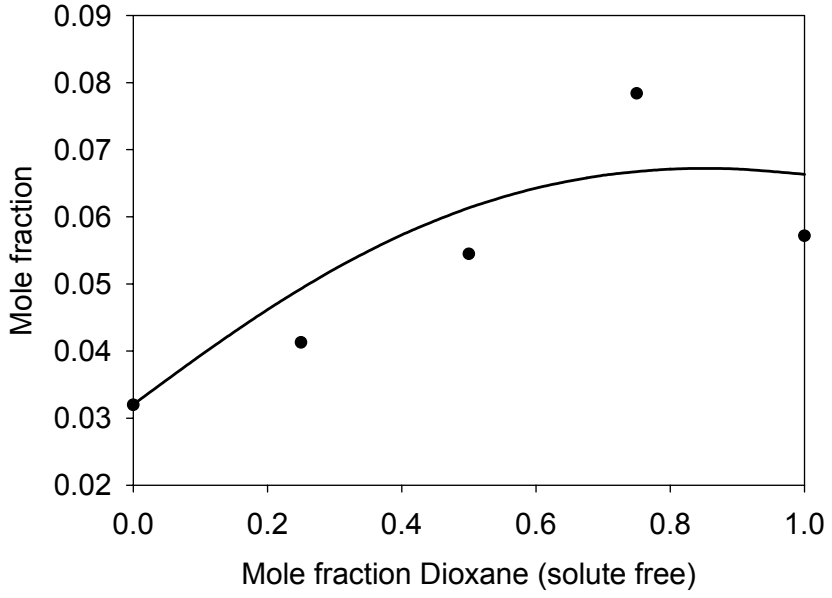


Figure 3-20. Solubility of 2-aminopyrimidine in dioxane/acetonitrile solvent mixtures at 298K.

the Wilson activity coefficient model is able to correctly predict the existence of a maximum in solubility in all the mixed solvents presented here, most accurately correlating the solubility in the methanol + nitromethane and methanol + acetonitrile binary solvent pairs. The prediction in the methanol + ethyl acetate mixed solvent is the poorest fit of the experimental data and is most likely due to the inaccuracy in the pure solvent solubility and not the mixed solvent characteristics.

For the example systems considered here, the accuracy of the predictions of the mixed solvent systems seems most dependent upon the correct prediction of the pure solvent solubilities and less dependent upon the accuracy of the binary solvent pair. In other words, when the pure solvent solubilities are predicted correctly the mixed solvent solubilties are predicted correctly. This may be because the MOSCED model has less average error for binary solvent predictions, and this error is less significant when compared to the larger error in the solid solubility predictions.

Summary

The solubility of four multi-functional solid compounds were measured in a variety of organic solvents at several temperatures and in several binary mixed solvents. The MOSCED model was successful at correlating the solubilities with few exceptions. The pure component descriptors were found to match the intuitive chemical/physical sense of the pure compounds. The model was also able to correctly predict the existence of maxima in solubility and at least qualitatively matches the experimental solubility.

The application of the MOSCED model to mixed solvent pairs is limited by the quality of the pure solvent predictions.

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CHAPTER IV

HIGH-PRESSURE VAPOR + LIQUID EQUILIBRIA OF SOME CARBON DIOXIDE + ORGANIC BINARY SYSTEMS

Introduction

Carbon dioxide is an interesting process solvent because it is non-flammable, inexpensive, non-toxic and miscible with many organic solvents. There has been recent interest in the use of carbon dioxide as an anti-solvent for crystallization of dissolved solutes. The choice of solvent in an anti-solvent process is a key factor in controlling solubility of the solute and control of particle morphology and size (Reverchon, Caputo et al. 2003). Further, CO_2 -expanded solvents as a medium for homogeneously (Musie, Wei et al. 2001) and heterogeneously (Tschan, Wandeler et al. 2001; Gläser, Williardt et al. 2003) catalyzed reactions have the potential advantage of increasing solubility and enhancing mass transfer of gaseous reactants. Carbon dioxide can also aid in the recycle of homogeneous catalysts by effecting a phase split in miscible water-organic-catalyst systems, as discussed in Chapter III in more detail.

All of these applications require knowledge of the vapor-liquid phase behavior and density of the carbon dioxide and organic solvent system, to select the most suitable solvent system and optimum operating conditions. To this end, vapor-liquid equilibria of

CO_2 + several organic solvents of industrial interest and of varying structure and polarity were measured to develop an understanding of the behavior of CO_2 in solution.

A recent review of high-pressure phase equilibria of Dohrn (Christov and Dohrn 2002) summarizes the data and techniques available. There are two main classes of experimental methods that are used to determine high-pressure phase equilibria, analytical (or direct sampling) and synthetic. Analytical methods involve using some type of physical or chemical detection system to determine equilibrium phase composition, usually involving the removal of a sample from the equilibrium cell. Some typical problems associated with this technique involve disturbing the equilibrium conditions, especially near condition sensitive critical regions, and possibly preferentially sampling the more volatile component. Direct sampling methods are either done statically, with either constant volume or variable volume equilibrium cells, or are dynamic methods, where the equilibrium phase(s) are flowing either in a recirculation path or are continuously flowing out of the equilibrium cells. In addition, calibration of the physiochemical detection apparatus is often time consuming and can be eliminated by using a synthetic technique.

A synthetic method avoids the problems of direct sampling by only observing the phase behavior of a known composition in the equilibrium cell. This can be accomplished by observing the incipient phase change, i.e. formation of the bubble-point in VLE, cloud-point in LLE, etc. or by using the material balances and measuring the volumes of all the equilibrium phases. Synthetic methods do require high pressure apparatus with view windows or transparent materials and some inexpensive cells are

readily available, like the Jerguson boiler gauges used in this study. They generally allow for quick composition determination with simple and easy experimental procedures.

The method presented here is a visual synthetic method that allows for quick and facile measurement of the VLE and PVT properties of mixtures of dense gases + organic solvents. The binary vapor-liquid equilibrium and liquid density of CO_2 + acetone, acetonitrile, dichloromethane, nitromethane, N-methyl-2-pyrrolidone, perfluorohexane, 2-propanol, tetrahydrofuran, toluene, and 2,2,2-trifluoroethanol were measured at temperatures from 298.2 K to 333.2 K. The data were correlated with the Patel-Teja cubic equation of state (PT-EoS) (Patel and Teja 1982) with the Matthias-Klotz-Prausnitz mixing rules (Mathias, Klotz et al. 1991).

Experimental Materials

HPLC grade 2-propanol (99%), acetone (99.9%), acetonitrile (99.9%), dichloromethane (99.9%), nitromethane (99%), N-methylpyrrolidone (99%), tetrahydrofuran (99.9%), toluene (99.9%), 2,2,2-trifluoroethanol (98%) and perfluorohexane (99.8%) were obtained from Aldrich Chemical Co. and were used as received. SFC Grade carbon dioxide (99.99%) was obtained from Matheson Gas Products. The CO_2 was further purified to remove trace water using a Matheson (Model 450B) gas purifier and filter cartridge (Type 451).

Apparatus and Procedures

Experimental Apparatus

Figure 4-1 shows a schematic of the equilibrium cell apparatus. The equilibrium cell is a transmission type sight gauge (Jerguson Model 18T-32). The working volume of the cell is 150 cm^3, which was measured by adding a known amount of gas to the cell at constant temperature and measuring the resulting pressure. The incremental volume scale on the sight gauge was calibrated by adding known volumes of water and measuring the resulting height to the nearest $1/16^{th}$ inch using the fixed scale and measuring any additional height less than the $1/16^{th}$ mark using a cathetometer readable to 0.0005 cm. The equilibrium cell was placed in a temperature controlled air bath. The temperature of the air bath and vapor phase inside the cell was monitored with a thermocouple (Omega Type K) and digital readout (HH-22 Omega). The air bath temperature was maintained by a digital temperature controller (Omega CN76000) with an over temperature controller (Omega CN375) for safe operation. The temperature was accurate to within ±0.2 K and calibrated against a platinum RTD (Omega PRP-4) with a DP251 Precision RTD Benchtop Thermometer (DP251 Omega) accurate to ±0.025 K and traceable to NIST. The pressures were measured with a pressure transducer and digital read-out (Druck, DPI 260, PDCR 910). The transducer was calibrated against a hydraulic piston pressure gauge (Ruska) to an uncertainty of +/- 0.1 bar. The cell is mounted on a rotating shaft, and mixing is achieved by rotating the entire cell.

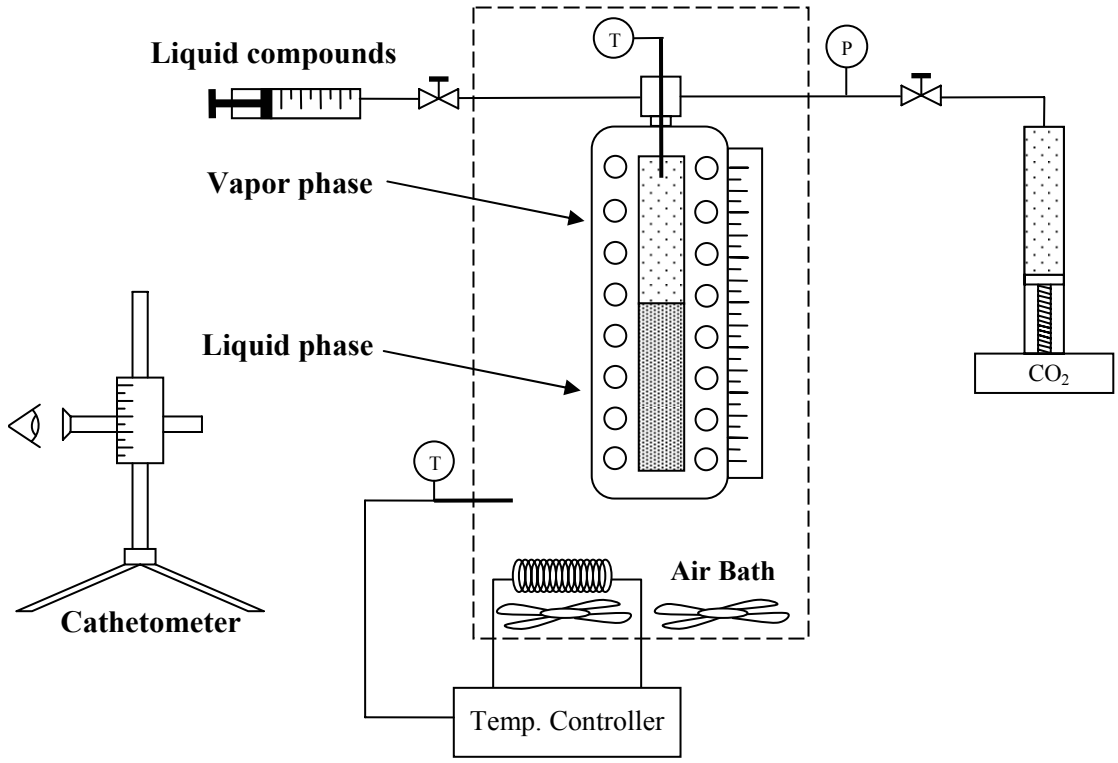


Figure 4-1. Schematic of equilibrium cell apparatus.

Experimental Procedure

After the cell was evacuated, the liquid compounds are added to the cell using a gas-tight syringe. The syringe was weighed before and after liquid addition to find mass added. CO_2 was added to the cell from a syringe pump (Isco Model 260D) operating at a constant pressure and temperature. The moles of CO_2 are determined from the volume displacement of the syringe pump and the density calculated from the Span-Wagner EoS (Span and Wagner 1996). The liquid volume was calculated by measuring the height of the meniscus with a fixed rule and the differences with a micrometer cathetometer. For displacements less than 50 mm, the accuracy is 0.01 mm; for larger displacements, the accuracy is 0.1 mm. The error in volume measurement is estimated to be ± 0.2 mL.

The composition of the liquid phase was found from the measured volume of the vapor phase, the total volume of the cell, and a calculated vapor phase composition and density using the Patel-Teja EoS (PT-EoS). The PT-EoS, shown in equation 4-1, was chosen because the volume translational term, *c*, gives a more accurate prediction of molar volume than Peng-Robinson or Soave-Redlich-Kwong equations. (Patel and Teja 1982)

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+c(v-b)} \qquad \text{Eq. 4-1}$$

The pure component parameters *a*, *b*, and *c* are given by equations 4-2 through 4-6,

$$a = \Omega_a \frac{R^2 T_c^2}{P_c}\left[1 + F\left(1 - \left(\frac{T}{T_c}\right)^{1/2}\right)\right]^2 \qquad \text{Eq. 4-2}$$

$$b = \Omega_b \frac{RT_c}{P_c} \qquad \text{Eq. 4-3}$$

$$c = \left(1 - 3\zeta_c\right)\frac{RT_c}{P_c} \qquad \text{Eq. 4-4}$$

where Ω_b is the smallest positive root of the cubic,

$$\Omega_b^3 + \left(2 - 3\zeta_c\right)\Omega_b^2 + 3\zeta_c^2\Omega_b - \zeta_c^3 = 0 \qquad \text{Eq. 4-5}$$

$$\Omega_a = 3\zeta_c^2 + 3\left(1 - 2\zeta_c\right)\Omega_b + \Omega_b^2 + 1 - 3\zeta_c \qquad \text{Eq. 4-6}$$

where P is pressure, T is temperature, R is the universal gas constant, v is molar volume, T_c is the critical temperature, and P_c is the critical pressure. The pure component parameters F and ζ_c are fit to the vapor pressure data and molar volume of that component. All pure component data are shown in Table 4-1.

The Mathias-Klotz-Prausnitz (MKP) mixing rules with two binary interaction parameters, as shown in equations 4-7 and 4-8, was used for mixture calculations.

$$a = \sum_i x_i \sum_j x_j a_{ji}^{(0)}\left(1 - k_{ji}\right) + \sum_i x_i \left(\sum_j x_j \left(a_{ji}^{(0)} l_{ji}\right)^{1/3} \right)^3 \qquad \text{Eq. 4-7}$$

$$\text{where,} \qquad a_{ji}^{(0)} = \sqrt{a_i a_j} \qquad \text{Eq. 4-8}$$

A two parameter mixing rule was necessary to model the phase behavior in the non-ideal alcohol + carbon dioxide systems studied. For all binary pairs, $k_{ij} = k_{ji}$ and $l_{ij} = -l_{ji}$. The following temperature dependency of the interaction parameters is used:

$$k_{ij} = k_{ij}^{(0)} + k_{ij}^{(1)} / T \qquad \text{Eq. 4-9}$$

$$l_{ij} = l_{ij}^{(0)} + l_{ij}^{(1)} / T \qquad \text{Eq. 4-10}$$

Linear mixing rules were used for parameters *b* and *c*, as shown in equations 4-11 and 4-12.

$$b = \sum_i x_i b_i \qquad \text{Eq. 4-11}$$

$$c = \sum_i x_i c_i \qquad \text{Eq. 4-12}$$

For the method presented here the calculation proceeds as follows: the mole fraction of the liquid phase is first estimated from the liquid phase volume expansion and used to calculate the bubble pressure, vapor composition, and vapor molar volume. The experimental volume of the vapor phase is related to the total moles in the vapor phase by equation 4-13, where $V_{\exp}^{V}$ is the measured volume of the vapor phase, $\bar{v}_{EoS}^{V}$ is the calculated molar volume of the vapor phase, and n^{V} is the total number of moles in the vapor phase. The composition of the liquid phase is the difference in total moles of component one (n_1^{tot}) and the moles of component 1 in the vapor phase, as shown by equation 4-14. The mole fractions of the liquid phase input into the bubble pressure

$$\frac{V_{\exp}^{V}}{\bar{v}_{\mathrm{EoS}}^{V}} = n^{V} \qquad \text{Eq. 4-13}$$

$$n_1^{tot} - y_1^{\mathrm{EoS}} n^{V} = n_1^{L} \qquad \text{Eq. 4-14}$$

calculation are varied using a simplex algorithm until input and output mole fractions agree. Block diagrams of the algorithm used for both the bubble pressure calculation and the calculation of the liquid composition are shown in Figures 4-2 & 4-3.

Figure 4-2. Block diagram for the calculation of the bubble-point pressure and vapor composition

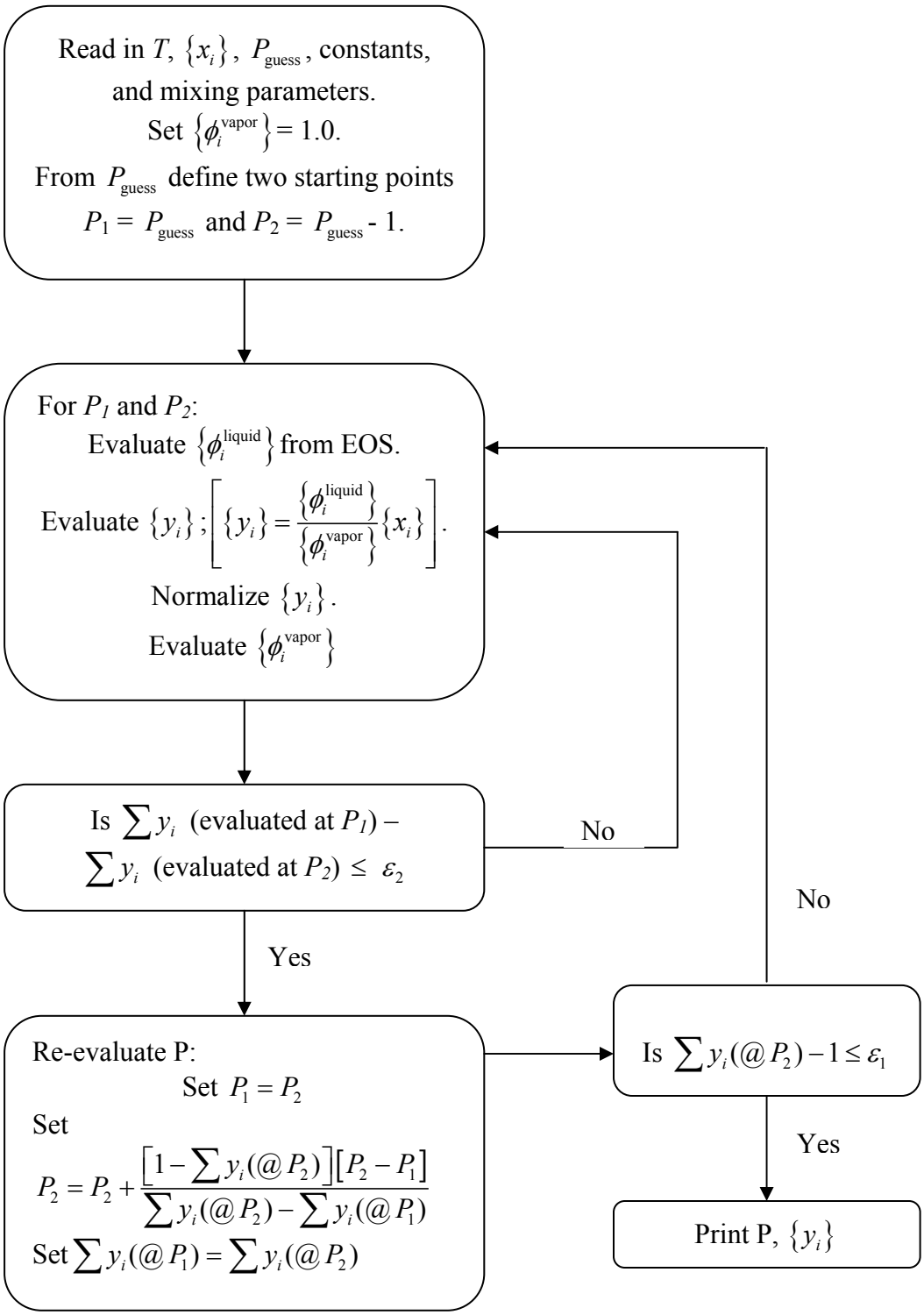
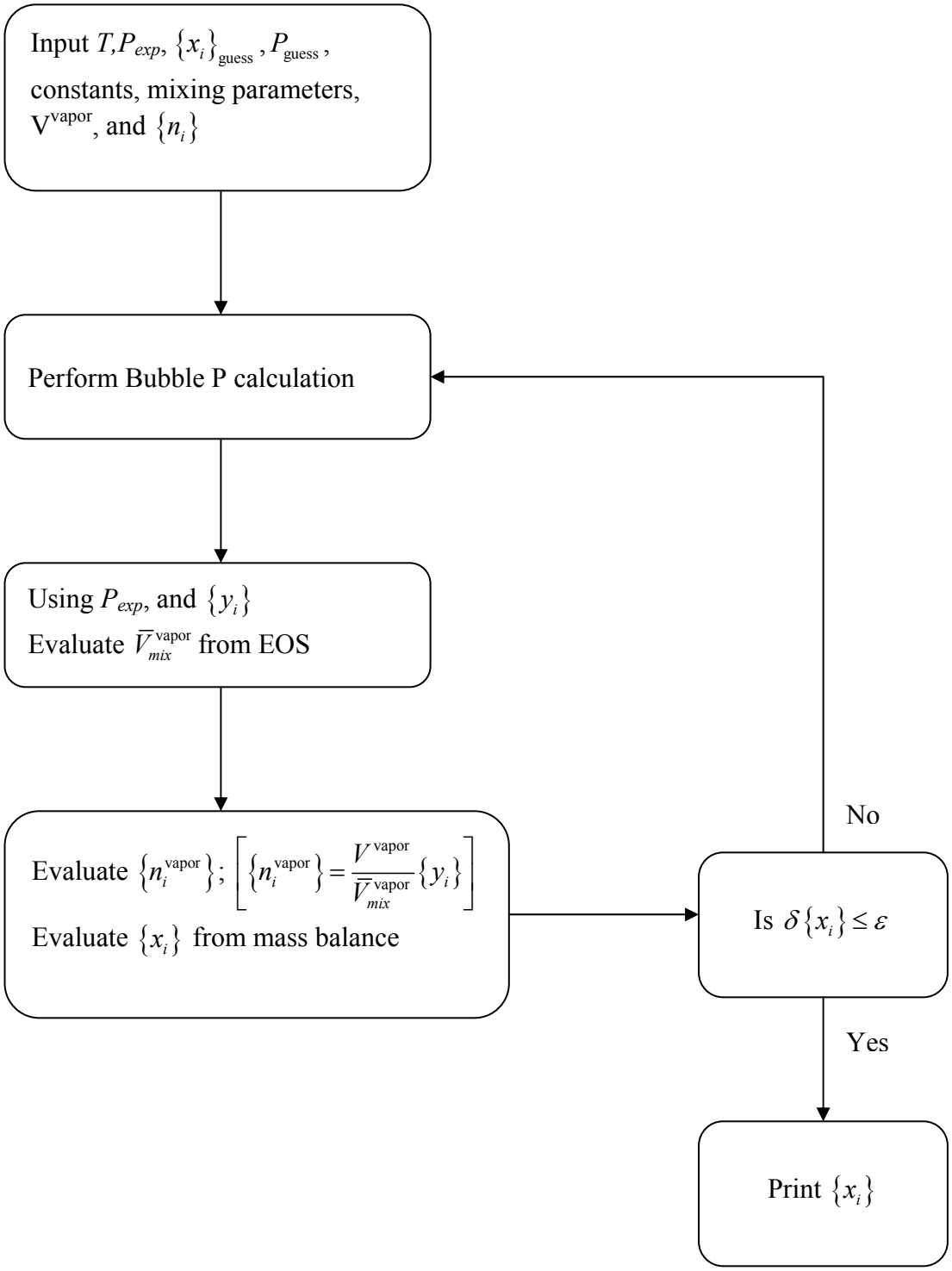


Figure 4-3. Block diagram for evaluation of liquid phase composition from measured volume, pressure, and mass.



The method presented here is similar to previously published visual synthetic techniques, where typically the vapor phase is assumed to contain none of the organic component and density or volume of the liquid phase is measured (Elbaccouch, Bondar et al. 2003) (Scurto, Lubbers et al. 2001). For the solvents in this study, the composition in the vapor phase was small but appreciable in the liquid phase composition.

The vapor phase composition is relatively independent of pressure in the range studied and independent of interaction parameters as shown in Figure 4-4. The mixing parameters were varied by ± 0.05 for the acetone + carbon dioxide system at 323 K. The effect of this change in the mixing parameters on the calculation of the liquid phase composition is less than 0.5% for the pressure range studied. Also, it can be seen that the PT-EoS prediction of the vapor phase composition is in good agreement with the data of Bamberger (Bamberger and Maurer 2000).

The molar volume of the liquid phase ($\bar{v}^L$), in equation 4-15, is found from the experimentally measured volume of the liquid phase (V^L_{exp}) and the total moles in the liquid phase ($n_1^L + n_2^L$) found from the above calculations.

$$\frac{V^L_{\text{exp}}}{n_1^L + n_2^L} = \bar{v}^L \qquad \text{Eq. 4-15}$$

The volume expansion of the liquid phase is defined as the change in total volume divided by the volume of the pure organic solvent liquid, as shown in equation 4-16.

$$\frac{V^L_{\text{exp}} - V^L_{\text{pure organic}}}{V^L_{\text{pure organic}}} \times 100 = \Delta V\% \qquad \text{Eq. 4-16}$$

Table 4-1. Pure component parameters used in the Patel-Teja CEoS. Critical temperature and pressure from the DIPPR database. ζ_c and F calculated to match density and vapor pressure data taken from the DIPPR database.

Compound	T_c (K)	P_c (MPa)	ζ_c	F
Acetone	508.2	4.70	0.2819	0.7085
Acetonitrile	545.5	4.83	0.2240	0.4780
Carbon Dioxide	304.2	7.36	0.3106	0.7115
Dichloromethane	510	6.08	0.2950	0.6320
Nitromethane	588.2	6.31	0.2633	0.6593
N-methyl-2-pyrrolidone	721.6	4.52	0.2768	0.7536
Perfluorohexane	451	1.86	0.3160	1.1185
2-Propanol	508.3	4.76	0.3001	1.2814
Tetrahydrofuran	540.2	5.19	0.3112	0.7266
Toluene	591.8	4.11	0.3080	0.7708
2,2,2-Trifluoroethanol	499	4.87	0.2952	1.2229

Table 4-2. Binary interaction parameters for CO_2 + Organic for MKP with Patel-Teja EoS.

Compound	$k_{ij}^{(0)}$	$k_{ij}^{(1)}$, K	$l_{ij}^{(0)}$	$l_{ij}^{(1)}$, K
Acetone	-0.005	--	0	--
Acetonitrile	-0.043	--	-0.074	--
Dichloromethane	0.046	--	0	--
Nitromethane	0.098	-33	0.318	-102
N-methyl-2-pyrrolidone	-0.012	--	0.005	--
Perfluorohexane	0.057	--	-0.069	--
2-Propanol	0.119	--	0.030	--
Tetrahydrofuran	0.137	-40	0.560	-173
Toluene	0.114	--	0.094	--
2,2,2-Trifluoroethanol	0.156	-28	0.373	-122

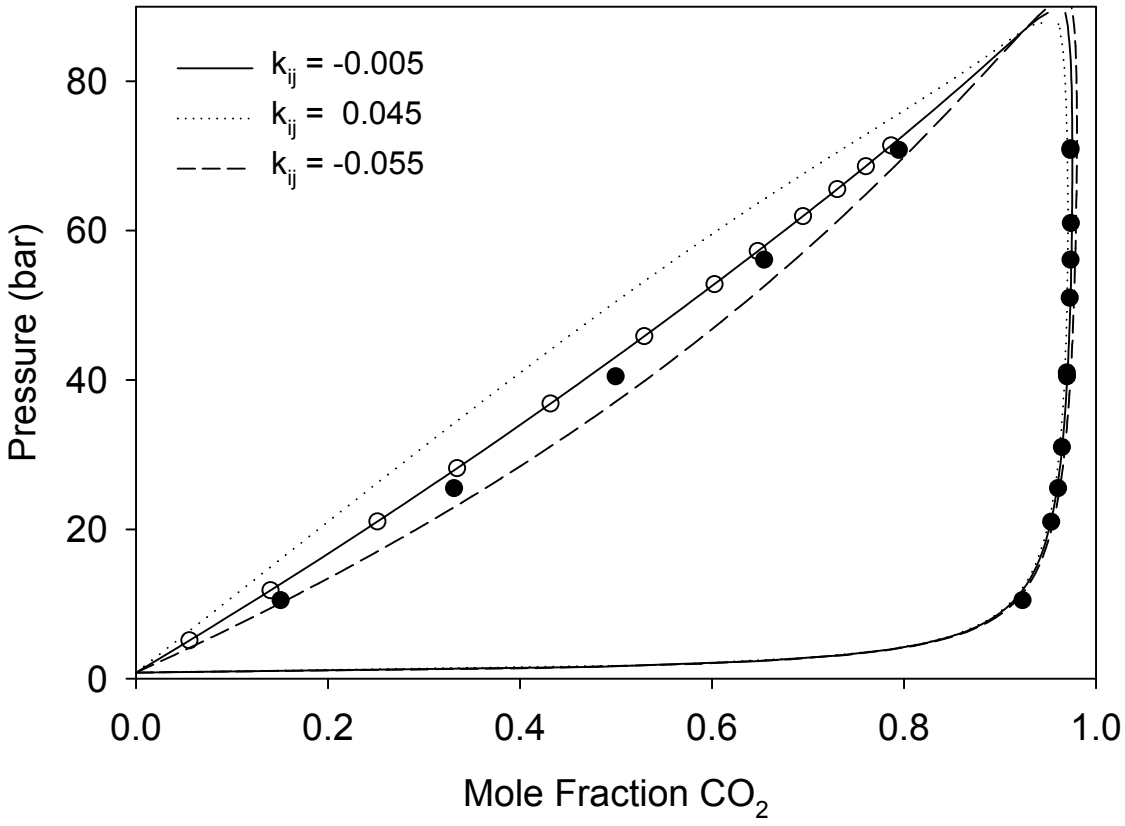


Figure 4-4. Vapor composition of CO_2 + Acetone vs. Pressure at 323 K. (○) this work, (●) data of Bamberger and Maurer(Bamberger and Maurer 2000) at 323 K, and lines are the Patel-Teja EoS bubble and dew curve correlations with different Van der Waals mixing parameters.

Results and Discussion

The binary vapor-liquid equilibrium and liquid density of CO_2 + acetonitrile, dichloromethane, N-methyl-2-pyrrolidone, perfluorohexane, and 2-propanol were measured at 313.2 K, CO_2 + nitromethane and CO_2 + 2,2,2-trifluoroethanol at 298.2 K and 313.2 K, CO_2 + tetrahydrofuran at 298.2 K, 313.2 K, 333.2 K, and CO_2 + acetone and CO_2 + toluene at 323.2 K. The data are shown in tables 4-3 to 4-16. The VLE data using the technique described here for the CO_2 + THF binary as shown in Figure 4-5, are in good agreement with recently published data of Im. (Im, Lee et al. 2004)

The binary interaction parameters for the MKP mixing rules are shown in Table 4-2. The binary interaction parameters were fit to minimize the difference between the pressure from the bubble pressure calculation and the experimental pressure.

Considering the solubility of CO_2 in a series of polar organic solvents as shown in Figure 4-6, some interesting behavior can be seen and insight into the nature of carbon dioxide in solution can be gleaned. The solubility of CO_2 at an arbitrary pressure of 50 bar is from most soluble to least soluble: perfluorohexane, tetrahydrofuran, dichloromethane, acetonitrile, N-methyl-2-pyrrolidone, nitromethane, 2,2,2-trifluoroethanol, 2-propanol. We will consider this solubility ordering below.

The high solubility of carbon dioxide in perfluorohexane is expected since it is known to be very soluble in fluorinated compounds. It is known that fluorocarbons have significantly larger ionization potentials than hydrocarbons (Reed 1955). As a consequence, the dispersion forces in fluorocarbons are substantially weaker than in hydrocarbons. No specific interactions are possible between carbon dioxide and

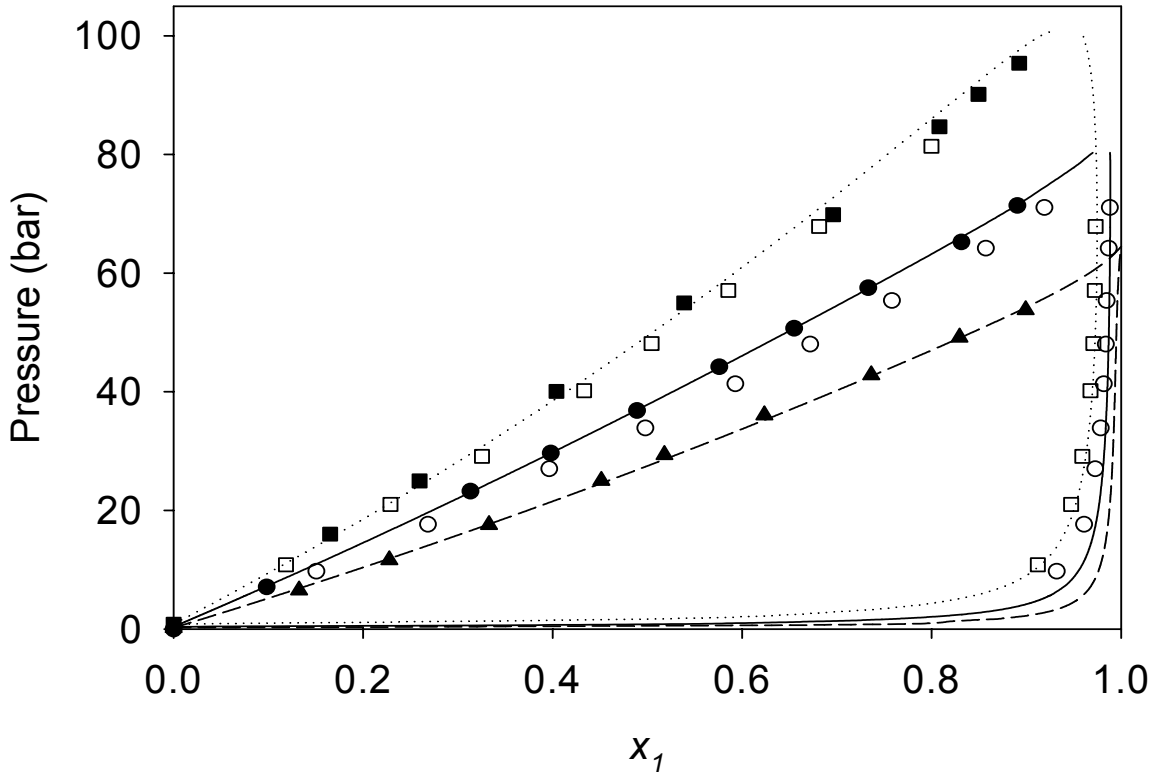


Figure 4-5. Comparison of P-x-y diagram of the CO_2 (1) + Tetrahydrofuran (2) system. 298 (▲), 313 (●), 333 (■), this work; 311.01(○), 331.33(□),(Im, et al.)(Im, Lee et al. 2004); lines are the Patel-Teja EoS.

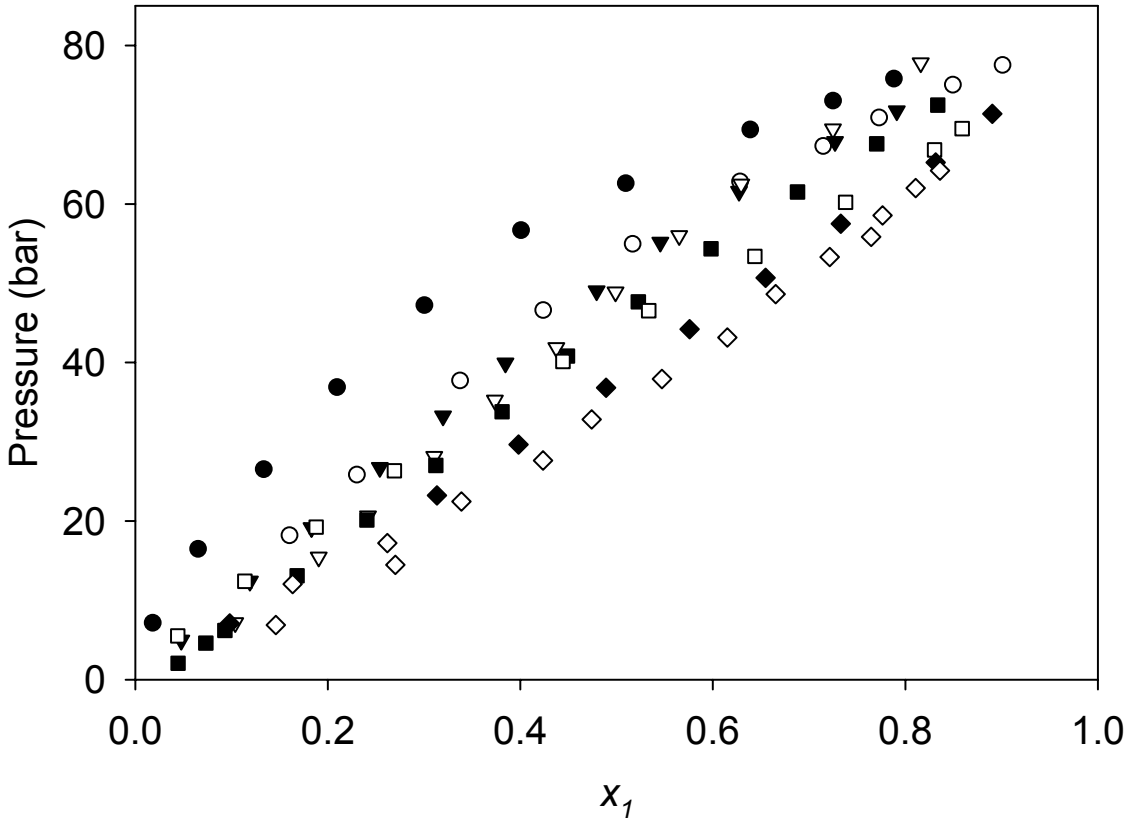


Figure 4-6. P-x-y diagram of the CO_2 (1) + Organic Solvents (2) at 313 K. 2-Propanol (●), TFE (○), Nitromethane (▼), NMP (▽), Acetonitrile (■), Dichloromethane (□), THF (◆), Perfluorohexane (◇).

perfluorohexane, therefore carbon dioxide must be of similar dispersion forces to account for high solubility.

Although CO_2 has a zero net dipole moment, it is not a non-polar species but does have a quadrupole moment. This allows for some charge separation on the carbon dioxide molecule, thus the electron deficient carbon atom can act as a Lewis acid or electron pair acceptor and the oxygen can act as weak electron pair donors. Kazarian and co-workers (Kazarian, Vincent et al. 1996) have shown through FT-IR and ATR-IR spectroscopy that the bending modes of carbon dioxide are affected by electron donating species. Carbonyl moieties were shown to have specific intermolecular interactions with CO_2 in an electron donor-electron acceptor complex. Raveendran and Wallen (Raveendran and Wallen 2002), through *ab initio* calculations, have shown that in addition to the carbon of CO_2 acting as a Lewis acid there is weaker but still significant interaction between the oxygen of CO_2 and a C-H moiety, which is termed to be a type of hydrogen bond. Kilic and co-workers (Kilic, Michalik et al. 2003) have further shown with some phase behavior studies with ab initio calculations that ether functionalities also can participate in specific interactions with CO_2.

We can thus postulate that the high solubility of tetrahydrofuran, is most likely due to some specific interactions with carbon dioxide. If we compare two solvents of the similar structure and the same polarizability/dipolarity but differing basicity, this behavior can be demonstrated. THF has a similar Kamlet-Taft solvatachromic polarizability/dipolarity parameter to that of benzene ($\pi^* = 0.58$ to $\pi^* = 0.59$). Comparing the solubility of CO_2 in THF to its solubility in benzene, we see a higher

solubility in THF, as can be seen in Figure 4-7. This is consistent with CO_2 is acting as a Lewis acid and interacting with the basic ether functionality of THF, and less so with the similarly structured and much less-basic aromatic ring of benzene. The carbon dioxide + 1,4-dioxane system exhibits similar behavior to the tetrahydrofuran system, which is consistent with the view of carbon dioxide acting as an acid in solution.

The high solubility of carbon dioxide in polar solvents like acetonitrile and nitromethane could attribute some dipolar character to it. There are two possible explanations for this behavior: one, the structure of carbon dioxide changes in solution, going from a linear molecule to one that is bent, or two, although there is no dipole moment, the bond poles of each C=O bond favorably interact with polar solvents in solution. There is some evidence that carbon dioxide does bend in interactions with polar moieties (Raveendran and Wallen 2002), however the change in polarity is not enough to account for strong dipole-dipole interactions. The favorable interactions of CO_2 with polar species in solution could be due to the electron donor ability or Lewis basicity present in most polar solvents. Specific Lewis acid-Lewis base interactions are only one of the several factors that affect solubility. The low dispersion forces or cohesive energy density of CO_2 as discussed earlier will tend to make it less soluble in solvents with larger dispersion forces or polarizability which can be higher for dipolar solvents.

A solubility comparison of similarly structured solvents, such as ethanol versus 2,2,2-trifluoroethanol is shown in Figure 4-8. This reveals that CO_2 is less soluble in the less polar, hydrogen bonded solvent (ethanol) than the more polar, unassociated solvent

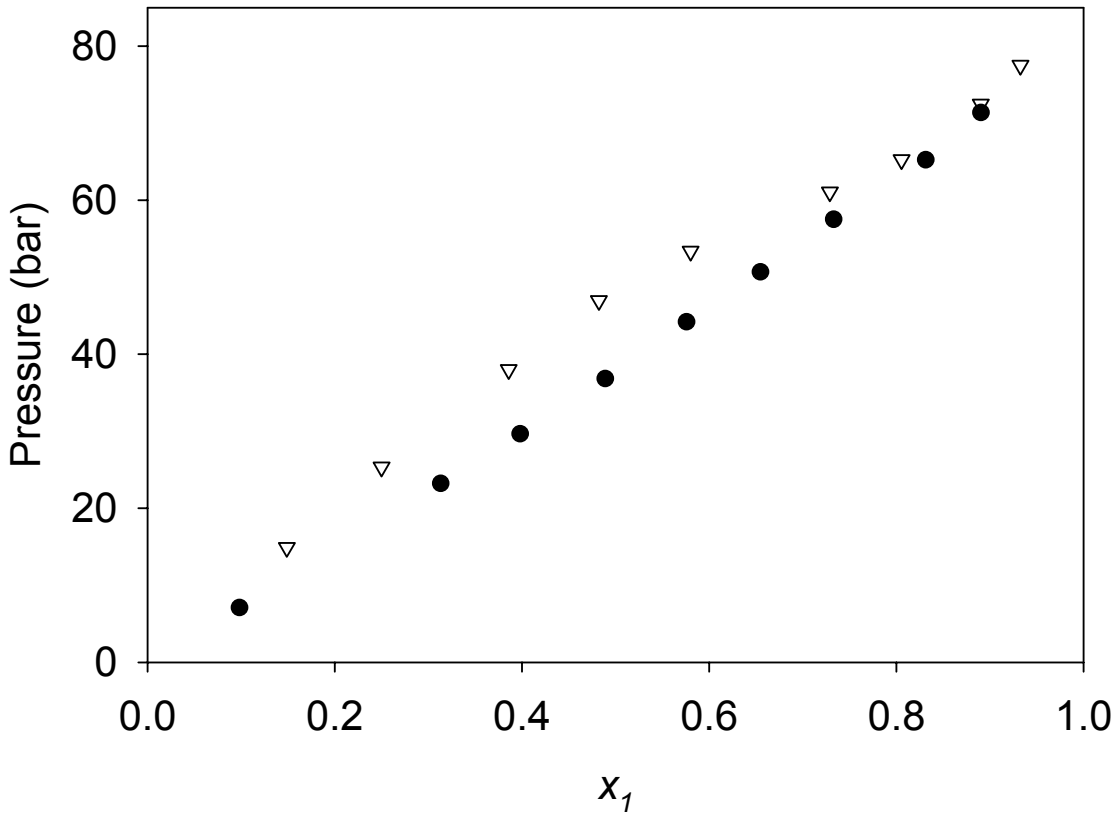


Figure 4-7. Comparison of P-x diagram of the CO_2 + tetrahydrofuran (●) (this work) and CO_2 + benzene (▽)(Ohgaki and Katayama 1976) at 313 K.

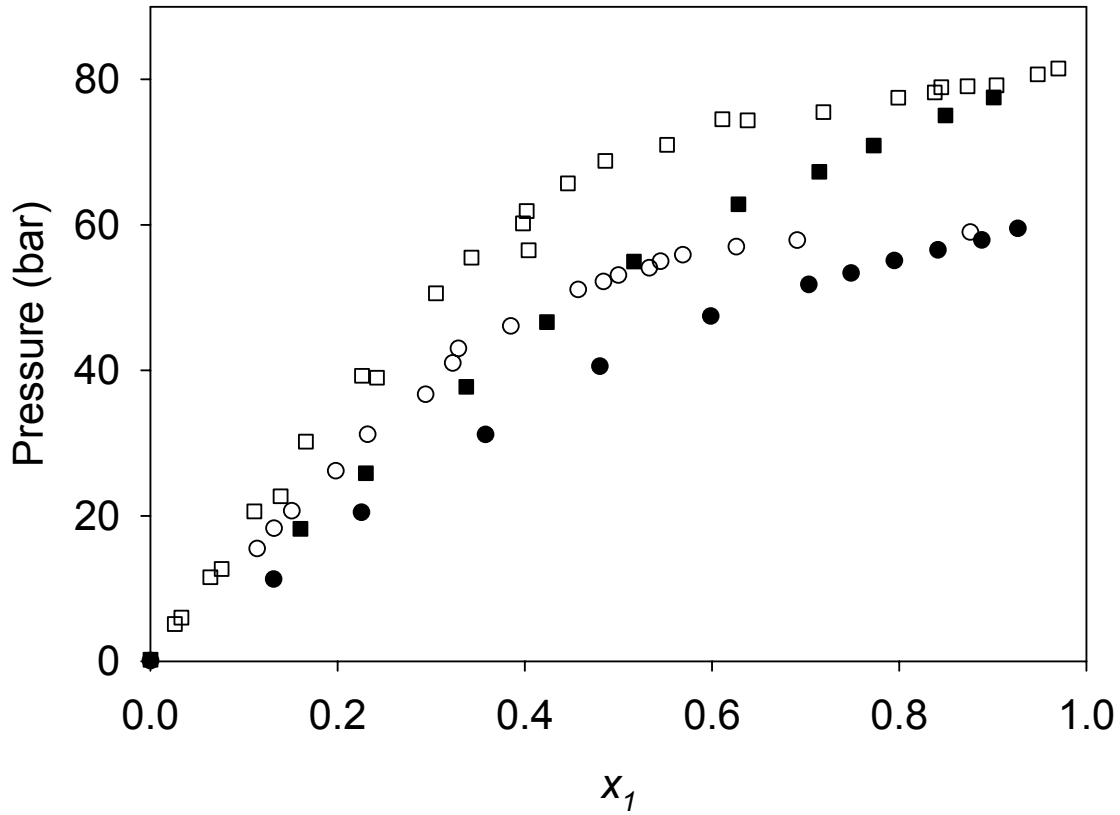


Figure 4-8. Comparison of the P-x diagrams of the CO_2 (1) + 2,2,2-Trifluoroethanol (2) system, at 298(●),313(■) and CO_2 (1) + Ethanol (2), at 298(○) (Kordikowski, Schenk et al. 1995), 313(□) (Suzuki, Sue et al. 1990),(Yoon, Lee et al. 1993), (Jennings, Lee et al. 1991).

(trifluoroethanol). The lack of solubility of carbon dioxide in solution indicates that it is not acidic enough to interrupt the hydrogen bond network in the ethanol system.

The change in volume to an organic solvent upon the addition of CO_2 is obviously dependent upon the density of the solvent. As can be seen in Figure 4-9, the rate of volume expansion versus weight fraction of CO_2 in the liquid phase is most rapid with very dense solvents like perfluorohexane (1.67 g/cm^3), less so with dichloromethane (1.29 g/cm^3) and slowest with acetonitrile (0.76 g/cm^3). If we assume that carbon dioxide adds at the same density for most of the composition range, at a weight fraction of 50%, a solvent with the same density as that of carbon dioxide would be expanded exactly 100%. From the plot we can see that the density that carbon dioxide in solution would be between that of nitromethane (1.13 g/cm^3) and tetrahydrofuran (0.89 g/cm^3). This agrees with Francis (Francis 1954) that CO_2 tends to add to organics liquids with a partial molar density of around 1.0 to 1.1 g/cm^3.

The partial molar volume at infinite-dilution of component 1 in a binary mixture is given by equation 4-17.

$$\bar{v}_1^{\infty} = v + (1 - x_1)\left.\frac{dv}{dx_1}\right|_{x_1=0} \qquad \text{Eq. 4-17}$$

Thus the intercept of the line of slope dv/dx_1 at a composition of pure component 1 (x_1 = 1) will give the partial molar volume of the component 1 in the solvent. The dilute region was assumed to be compositions less than 0.25 mole fraction carbon dioxide, and linear regression was used on this data to find the partial molar volume. The experimental molar volume data at 313 K along with the linear regressions are shown in Figure 4-10.

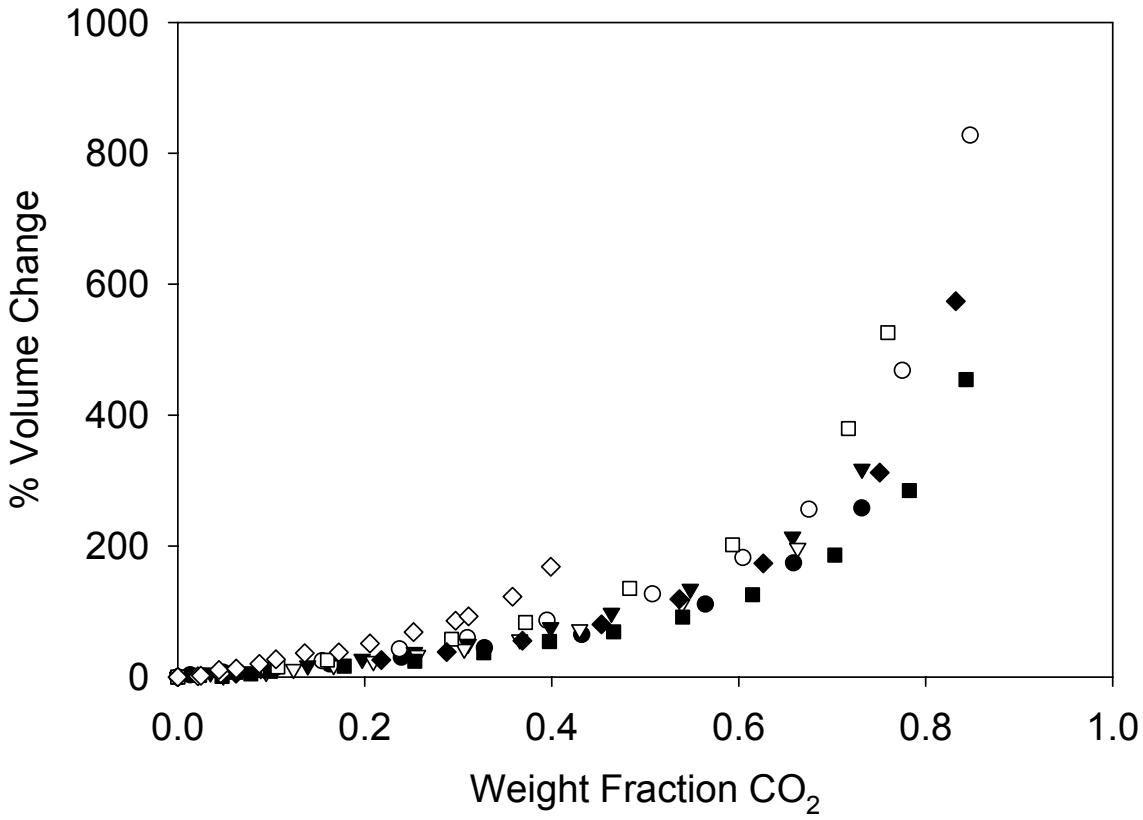


Figure 4-9. Percent volume change vs. weight fraction of CO_2 of the Carbon Dioxide + Organics at 313 K. 2-Propanol (●), TFE (○), Nitromethane (▼), NMP (▽), Acetonitrile (■), Dichloromethane (□), THF (◆), Perfluorohexane (◇).

All of the partial molar volume values for carbon dioxide in the polar solvents studied here are between 45 and 55 cm^3/mol. It is not possible to compare this molar volume to that of the liquid density of pure carbon dioxide because 313 K is above the critical temperature of CO_2. A comparison can be made at a high pressure where the molar volume is not sensitive to pressure changes. At 250 bar and 313 K the molar volume of CO_2 is around 48 cm^3/mol, which is in the range of the partial molar volumes of CO_2 in the liquid phases. Thus it can be concluded that the partial molar volume is similar to the molar volume of carbon dioxide in the pseudo-liquid state above the critical temperature. However, for the non-polar solvent perfluorohexane, the partial molar volume is much higher at 77 cm^3/mol. This difference could possibly result from the low dispersion energies of both components in the system, as previously discussed. At the lower saturation pressures of the solution, because of the lack of specific interactions, the partial molar volume of carbon dioxide would tend more towards the higher molar volumes of pure CO_2 at these conditions.

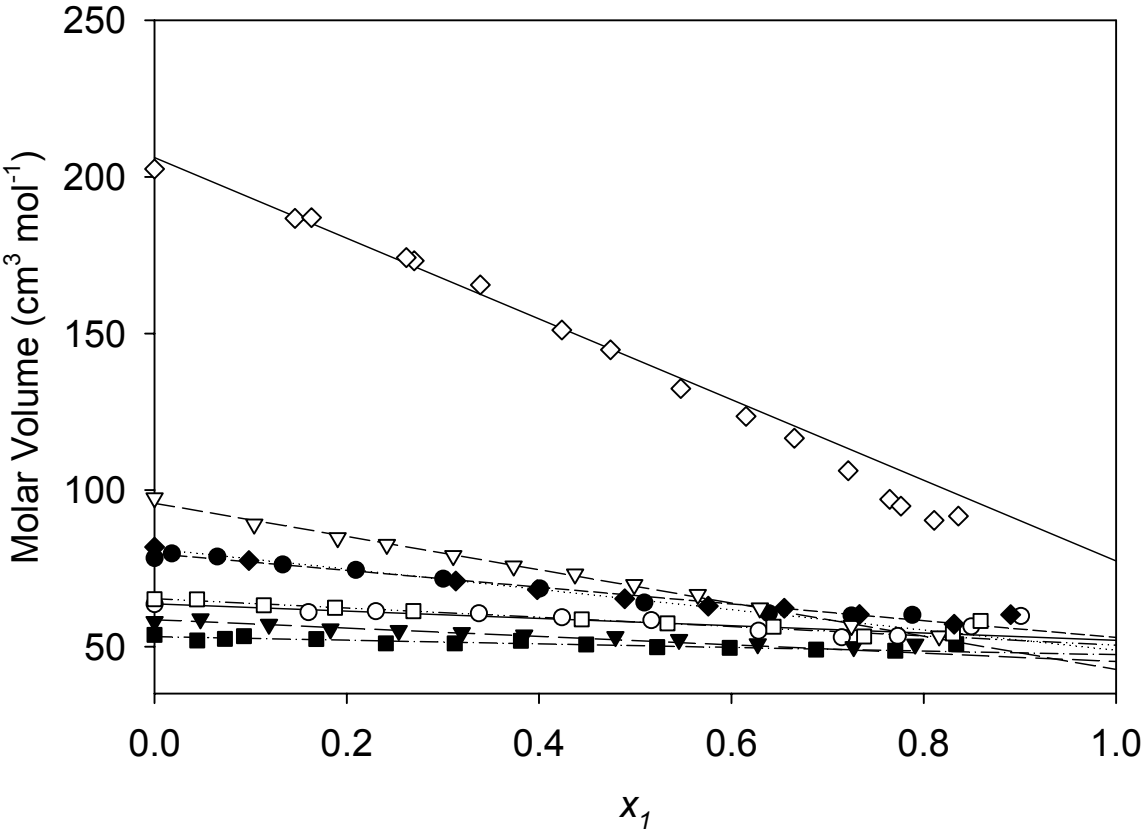


Figure 4-10. Molar Volume of the liquid phase vs. mol fraction of CO_2 of the Carbon Dioxide (1) + Organics (2) at 313 K. 2-Propanol (●), TFE (○), Nitromethane (▼), NMP (▽), Acetonitrile (■), Dichloromethane (□), THF (◆), Perfluorohexane (◇).

Summary

A visual synthetic method that allows for quick and facile measurement of the VLE and PVT properties of mixtures of dense gases + organic solvents is presented here. The binary vapor-liquid equilibrium and liquid density of CO_2 + acetone, acetonitrile, dichloromethane, nitromethane, N-methyl-2-pyrrolidone, perfluorohexane, 2-propanol, tetrahydrofuran, toluene, and 2,2,2-trifluoroethanol were measured at temperatures from 298.2 K to 333.2 K. The data were correlated with the Patel-Teja cubic equation of state with the Matthias-Klotz-Prausnitz mixing rules.

Insight into the specific interactions between carbon dioxide and the various organic solvents give insight into the nature of carbon dioxide in solution. Comparison of the P-x data indicate that carbon dioxide has low dispersion energy to explain the lower solubility in aromatic solvents, some dipolar character is consistent with the solubility in dipolar solvents, and some Lewis acidity to explain the high solubility in basic solvents, like acetone, which actually demonstrates negative deviations from ideality.

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Table 4-3. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + 2-Propanol system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		2-Propanol		
313		0	78.3	0%
313	7.2	0.018	79.7	3%
313	16.5	0.065	78.8	7%
313	26.6	0.133	76.2	12%
313	36.9	0.210	74.5	20%
313	47.2	0.300	71.7	30%
313	56.7	0.401	68.5	45%
313	62.6	0.510	64.0	65%
313	69.4	0.639	60.6	111%
313	73.0	0.725	59.9	174%
313	75.8	0.788	60.1	258%

Table 4-4. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Acetonitrile system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Acetonitrile		
313		0	53.8	0%
313	2.1	0.044	51.9	1%
313	4.6	0.073	52.5	5%
313	6.2	0.093	53.3	9%
313	13.1	0.168	52.4	16%
313	20.1	0.241	51.1	24%
313	27.0	0.312	51.0	37%
313	33.8	0.381	51.8	54%
313	40.8	0.449	50.7	69%
313	47.7	0.523	49.8	91%
313	54.3	0.598	49.6	126%
313	61.5	0.688	49.0	186%
313	67.6	0.770	48.7	285%
313	72.5	0.834	50.8	454%

Table 4-5. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Dichloromethane system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Dichloromethane		
313		0	65.1	0%
313	5.5	0.044	65.1	2%
313	12.4	0.114	63.2	7%
313	19.2	0.188	62.4	15%
313	26.3	0.269	61.3	26%
313	40.1	0.444	58.7	58%
313	46.6	0.533	57.4	83%
313	53.4	0.644	56.4	135%
313	60.2	0.738	53.2	202%
313	66.8	0.830	54.2	380%
313	69.5	0.859	58.2	526%

Table 4-6. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Nitromethane system at 298 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Nitromethane		
298		0	51.1	0%
298	8.9	0.120	49.3	9%
298	18.5	0.238	48.3	24%
298	26.9	0.346	47.6	42%
298	35.2	0.457	47.4	71%
298	41.4	0.552	47.4	107%
298	48.3	0.678	47.1	185%
298	51.4	0.747	47.7	267%
298	54.3	0.810	47.8	391%
298	55.7	0.855	48.7	558%
298	56.6	0.876	49.1	671%

Table 4-7. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Nitromethane system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Nitromethane		
313		0	58.0	0%
313	5.0	0.048	58.8	6%
313	12.4	0.119	57.1	12%
313	19.2	0.183	55.6	17%
313	26.8	0.254	55.1	27%
313	33.2	0.320	54.5	38%
313	39.9	0.385	53.7	50%
313	49.0	0.479	53.2	76%
313	55.2	0.546	52.3	98%
313	61.6	0.627	50.9	134%
313	67.9	0.727	49.9	214%
313	71.7	0.791	50.8	318%

Table 4-8. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + N-methyl-2-pyrrolidone system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		N-methyl-2-pyrrolidone		
313		0	97.5	0%
313	7.2	0.104	89.1	2%
313	15.4	0.190	84.8	7%
313	20.6	0.242	82.6	12%
313	28.1	0.311	79.0	18%
313	35.2	0.374	75.7	24%
313	41.9	0.437	73.2	33%
313	48.9	0.499	69.8	43%
313	56.0	0.565	66.6	57%
313	62.5	0.629	62.3	73%
313	69.4	0.725	56.7	111%
313	77.8	0.816	53.4	197%

Table 4-9. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Tetrahydrofuran system at 298 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Tetrahydrofuran		
298		0	78.2	0%
298	6.6	0.132	70.8	4%
298	11.7	0.228	65.5	8%
298	17.6	0.333	64.6	24%
298	25.0	0.451	62.0	44%
298	29.4	0.518	60.8	61%
298	36.1	0.624	58.6	98%
298	42.8	0.736	56.4	173%
298	49.2	0.830	54.9	312%
298	53.8	0.899	54.3	590%

Table 4-10. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Tetrahydrofuran system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Tetrahydrofuran		
313		0	81.8	0%
313	7.1	0.098	77.5	5%
313	23.2	0.313	70.9	26%
313	29.7	0.398	68.2	38%
313	36.8	0.489	65.3	55%
313	44.2	0.576	62.9	80%
313	50.7	0.655	62.3	119%
313	57.5	0.733	60.2	174%
313	65.2	0.832	57.2	312%
313	71.4	0.890	60.2	574%

Table 4-11. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Tetrahydrofuran system at 333 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Tetrahydrofuran		
333		0	78.9	0%
333	16.0	0.165	74.5	12%
333	25.0	0.260	73.4	24%
333	40.1	0.404	68.7	43%
333	55.0	0.539	66.0	76%
333	69.9	0.696	58.4	133%
333	84.7	0.808	60.4	272%
333	90.1	0.850	62.9	390%
333	95.4	0.893	70.5	690%

Table 4-12. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + 2,2,2-Trifluoroethanol system at 298 K.

T K	P bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		2,2,2-Trifluoroethanol		
298		0	67.6	0%
298	11.3	0.132	63.9	9%
298	20.5	0.225	63.0	20%
298	31.2	0.358	59.5	37%
298	40.6	0.480	58.1	65%
298	47.4	0.599	57.1	110%
298	51.8	0.704	55.1	174%
298	53.4	0.749	55.1	223%
298	55.1	0.795	54.3	290%
298	56.6	0.842	54.9	410%
298	57.9	0.888	54.8	624%
298	59.5	0.927	55.0	1014%

Table 4-13. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + 2,2,2-Trifluoroethanol system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		2,2,2-Trifluoroethanol		
313		0	63.5	0%
313	18.2	0.160	61.0	14%
313	25.9	0.230	61.3	25%
313	37.7	0.337	60.6	43%
313	46.6	0.424	59.4	60%
313	55.0	0.517	58.4	87%
313	62.8	0.628	55.1	127%
313	67.3	0.715	53.0	183%
313	70.9	0.773	53.4	256%
313	75.0	0.849	56.5	468%
313	77.5	0.901	59.8	828%

Table 4-14. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Perfluorohexane system at 313 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Perfluorohexane		
313		0	202.5	0%
313	6.9	0.146	186.7	1%
313	12.1	0.163	187.0	2%
313	14.5	0.270	173.2	5%
313	17.2	0.262	174.2	11%
313	22.5	0.339	165.5	13%
313	27.7	0.424	151.1	20%
313	32.8	0.474	144.8	27%
313	37.9	0.547	132.4	37%
313	43.2	0.615	123.5	38%
313	48.6	0.665	116.5	51%
313	53.3	0.721	106.2	68%
313	55.9	0.765	97.0	86%
313	58.6	0.776	94.9	93%
313	62.0	0.811	90.3	123%
313	64.2	0.836	91.7	168%

Table 4-15. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Acetone system at 323 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Acetone		
323		0	74.6	0%
323	4.9	0.056	73.7	4%
323	11.1	0.140	71.8	11%
323	20.0	0.251	67.5	19%
323	27.4	0.335	66.7	33%
323	36.3	0.432	64.2	49%
323	45.9	0.530	62.3	74%
323	53.6	0.603	61.0	102%
323	58.1	0.648	60.1	124%
323	63.0	0.695	57.1	146%
323	65.2	0.730	56.6	177%
323	67.8	0.760	57.4	216%
323	71.1	0.787	58.1	260%

Table 4-16. Composition, Pressure, Molar Volume, and Volume Expansion of the Carbon Dioxide + Toluene system at 323 K.

T K	*P* bar	x_{CO2}	v_L $cm^3\ mol^{-1}$	ΔV %
		Toluene		
323		0	109.3	0%
323	12.0	0.091	101.4	2%
323	21.2	0.175	97.2	7%
323	31.5	0.260	92.1	13%
323	40.1	0.335	87.6	19%
323	48.1	0.408	83.7	28%
323	55.4	0.480	80.2	39%
323	59.6	0.524	78.2	48%
323	63.1	0.583	72.2	55%
323	67.2	0.644	67.2	69%
323	73.8	0.715	64.6	101%
323	78.0	0.764	63.2	137%
323	82.1	0.821	62.3	206%
323	85.0	0.865	62.6	309%
323	86.6	0.883	63.5	383%

CHAPTER V

SOLUBILITY OF A PERMANENT GAS REACTANT IN A GAS-EXPANDED LIQUID

Introduction

There has been much recent interest in the use of supercritical or gaseous carbon dioxide in both heterogeneous and homogeneous catalyzed reactions. Replacing reaction solvents with carbon dioxide take advantage of its non-toxicity, miscibility with many organics, and ease of downstream separations. For reactions involving permanent gases (H_2, CO, O_2) carbon dioxide's miscibility with gaseous reactants above its critical temperature (304K) can remove phase boundaries and eliminate mass transfer limitations. Of particular interest are oxidation reactions, where because of the non-reactivity of carbon dioxide, no oxidation products are formed.

The dangers associated with using molecular oxygen as the oxidant could possibly be made safer because of the ability of carbon dioxide to inert otherwise flammable mixtures. Carbon dioxide is known to give smaller concentration regions of explosion/flammability than nitrogen or steam (Haessler 1989). It should be pointed out that high pressure does expand the flammability region for reactive mixtures (Holtappels, Brinkmann et al. 2001). For example, the explosion limit concentrations in the gaseous

phase for a mixture of ethylene/air with carbon dioxide as the inert diluent are roughly doubled in area when the pressure is increased from 1 bar to 100 bar, as shown in Figure 5-1. As long as high concentrations of carbon dioxide in the vapor phase are maintained the explosion limit concentrations can be avoided.

Subramaniam has also shown the high heat capacity of carbon dioxide lowers adiabatic temperature rise and could allow for better temperature control (Jin and Subramaniam 2003). At temperatures near the critical temperature, the heat capacity goes through a maximum, approximately four times greater than the heat capacity in the dense liquid-like region. As shown in Figure 5-2, the maximum in heat capacity coincides with the rapid change in density going from the vapor to liquid like densities. At the critical point, the density goes through rapid fluxuations, causing the phenomena of critical opalescence, and the heat capacity going to infinity. It is not surprising that at temperatures near the critical temperature, similar behavior is observed. For strongly exothermic reactions, operating at lower pressures near the critical temperature would improve the temperature control of the reaction and lessen the possibility of run-away reactions.

Replacing all the organic solvent and running a reaction in a single supercritical phase will eliminate any mass transfer that may occur across the vapor-liquid interface; this also makes the process more environmentally benign by eliminating the use of volatile organic compounds that can be released. Unfortunately, for many organic reactants, especially for high molecular weight compounds, there is minimal solubility in the super-critical solvent phase. However, as Beckman points out (Beckman 2004), the

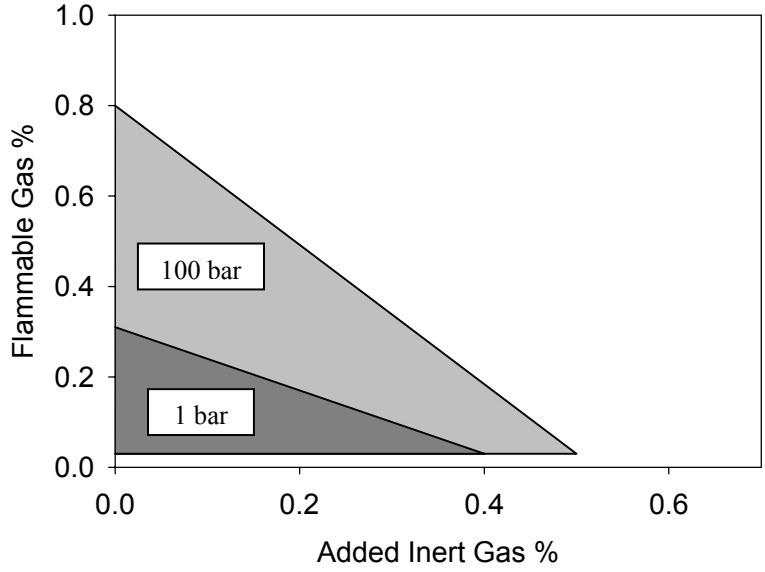

Figure 5-1. Approximate explosion limits for gaseous ethylene/CO_2/air mixtures at 303 K and pressures of 1 and 100 bar. Shaded areas represent explosive concentration range.

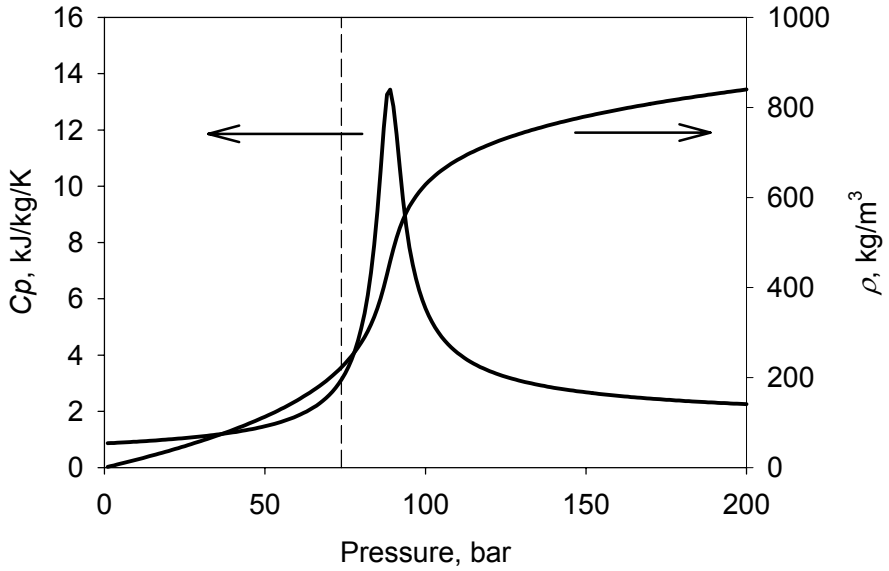

Figure 5-2. Density and heat capacity of CO_2 at 313 K as a function of pressure. Curves calculated from Span-Wagner EoS (Span and Wagner 1996).

addition of carbon dioxide to the liquid phase will enhance the solubility of gaseous reactants and allow operation at lower pressures and allow higher concentrations of reactants in the continuous phase. The use of gas expanded liquid solvents could also enhance product yield. Subramaniam has shown in the heterogeneously catalyzed oxidation of cyclohexene a maximum in yield using liquid mixtures of carbon dioxide and acetonitrile as the solvent (Kerler, Robinson et al. 2004). Understanding of the phase boundaries in the multi-component system must therefore be known to accurately describe the effect of the solvent system on the reaction (Jenzer, Schneider et al. 2001; Grunwaldt, Wandeler et al. 2003). The solubility of oxygen in the liquid phase will have a strong influence on the reaction rate and performance of the catalyst. In this work, we have chosen the oxidation of 2-propanol to acetone in the presence of oxygen as a model reaction system to investigate the solubility of oxygen in the carbon dioxide-expanded liquid phase and identify the single phase region as a function of total system pressure. The catalyzed oxidation of 2-propanol in supercritical carbon dioxide has been previously reported with consideration of the phase equilibria (Gläser, Williardt et al. 2003).

For the phase equilibria experiments we substituted argon for oxygen. Argon (T_c = 150.86 K , P_c = 48.98 bar) and oxygen (T_c = 154.6 , P_c = 50.46 bar) have similar critical properties and their Henry's constants are similar in organic solvents (Lühring and Schumpe 1989). The use of oxygen in the equilibria measurements was avoided because of the potential to form explosive mixtures in the large head-space present in the equilibrium vessel. In addition any slow formation of oxidation products can be avoided.

The high pressure phase vapor-liquid equilibria of CO_2 + Argon + 2-Propanol was measured at three pressures 6.9, 11.0, and 15.0 MPa at a constant temperature of 313 K. The data were correlated with the Patel-Teja Equation of State (Patel and Teja 1982) using the two parameter Mathias-Klotz-Prausnitz mixing rules (Mathias, Klotz et al. 1991).

The creation of water and other oxidation by-products, depending upon conversion, can significantly affect the phase equilibria of a reacting system. In the catalyzed oxidation of 2-propanol only acetone and water are formed in the reaction. This results in a 5-component system, where water, because of low gas solubility, has the potential to alter the phase boundaries. The effect of product formation on the solubility of argon was determined at 313 K and 6.9, 11.0, and 15.0 MPa.

Experimental Materials

HPLC grade 2-propanol (99%), acetone (99%), and water (99%) were obtained from Aldrich Chemical Co. and were used as received. Ultra-pure carrier grade Argon (99.9999%) was obtained from Air Products. SFC Grade carbon dioxide (99.99%) was obtained from Matheson Gas Products. The CO_2 was further purified to remove trace water using a Matheson (Model 450B) gas purifier and filter cartridge (Type 451).

Apparatus and Procedure

Apparatus

Figure 5-3 shows a schematic of the equilibrium cell apparatus. The equilibrium cell consists of a hollow sapphire cylinder (50.8 mm O.D. × 25.4±0.0001 mm I.D. × 203.2 mm L) with a movable stainless steel piston inside and stainless steel end caps. The cell is divided into two chambers separated by an O-ring seal on the piston, one side containing the equilibrium components and the other side containing the pressuring fluid, in this case water. The equilibrium cell was placed in a temperature controlled air bath. The temperatures of the air bath and vapor phase inside the cell were monitored with thermocouples (Omega Type K) and digital readouts (HH-22 Omega). The air bath temperature was maintained by a digital temperature controller (Omega CN76000) with an over temperature controller (Omega CN375) for safe operation. The temperature was accurate to within ±0.2 K and calibrated against a platinum RTD (Omega PRP-4) with a DP251 Precision RTD Benchtop Thermometer (DP251 Omega) accurate to ±0.025 K and traceable to NIST. The pressures were measured with a pressure transducer and digital read-out (Druck, DPI 260, PDCR 910). The transducer was calibrated against a hydraulic piston pressure gauge (Ruska) to an uncertainty of ± 0.01 MPa.

Liquid and vapor volumes are calculated by measuring the height of the meniscus with a micrometer cathetometer. For displacements less than 50 mm, the accuracy is 0.01 mm; for larger displacements, the accuracy is 0.1 mm. The cell is mounted on a rotating shaft, and mixing is achieved by rotating the entire cell.

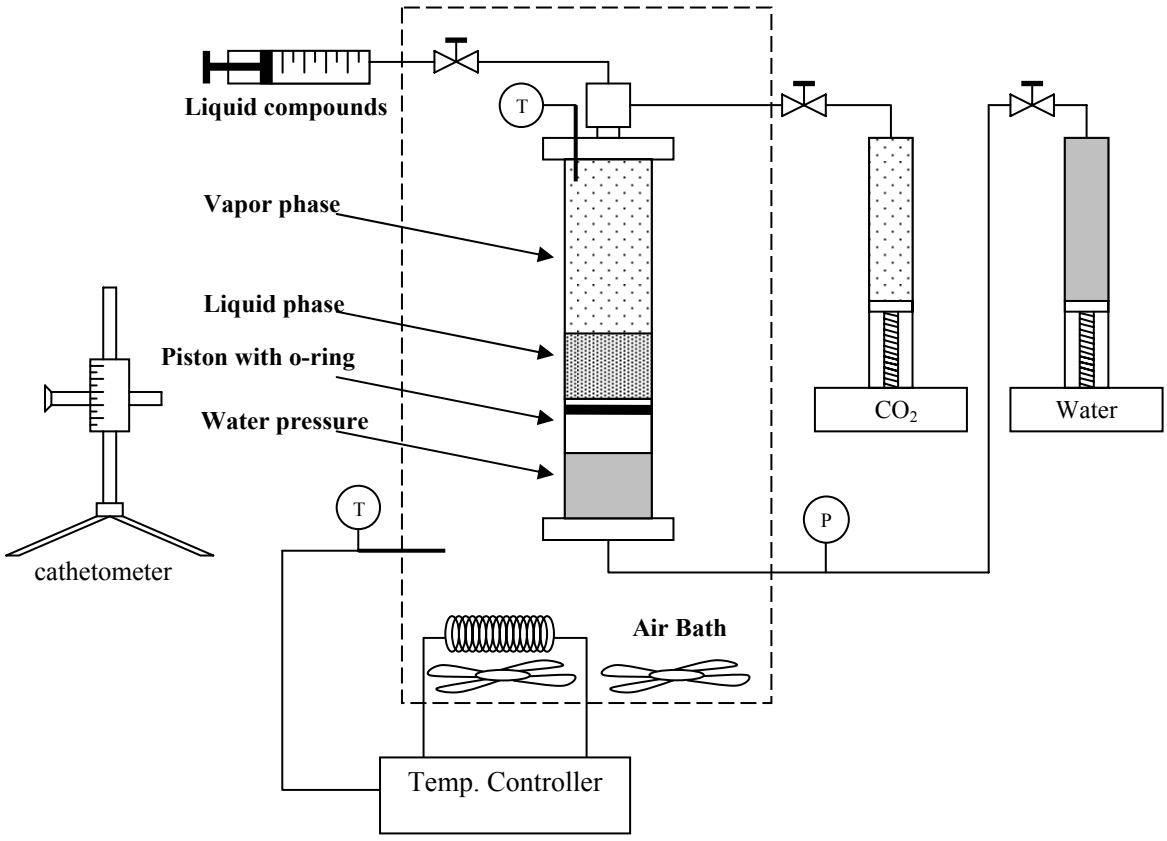

Figure 5-3. Schematic of equilibrium cell apparatus.

Experimental Procedure

The liquid phase compounds are added to the cell using a gas-tight syringe. The syringe was weighed before and after liquid addition to find mass added and had an estimated error of less than ±0.05 grams or less than ±0.1% of mass loaded. CO_2 was added to the cell from a syringe pump (ISCO, Inc., Model 500D) operated at a constant pressure and temperature. Using the volume displacement of the syringe and the highly accurate Span-Wagner EoS (Span and Wagner 1996), the moles of CO_2 added to the cell is calculated with an error of ± 0.001 moles, or for the smallest loading an error of ±1.5% in moles added. The loading of argon to the equilibrium cell was accomplished by using a high-pressure cell of known volume at a fixed temperature. The cell is loaded to a fixed pressure at a constant temperature. The change in pressure upon addition of argon to the equilibrium cell was monitored and using the equation of Tegeler, Span, and Wagner (Tegeler, Span et al. 1999) the moles added can be calculated.

The composition of the liquid phase was found from the measured volume of the vapor phase, the total volume of the cell, and a calculated vapor phase composition and density using the Patel-Teja EoS (PT-EoS). The PT-EoS, shown in equation 5-1, was chosen because the volume translational term, *c*, gives a more accurate prediction of molar volume than Peng-Robinson or Soave-Redlich-Kwong equations. (Patel and Teja 1982)

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+c(v-b)} \qquad \text{Eq. 5-1}$$

The pure component parameters *a*, *b*, and *c* are given by equations 5-2 through 5-6,

$$a = \Omega_a \frac{R^2 T_c^2}{P_c}\left[1 + F\left(1 - \left(\frac{T}{T_c}\right)^{1/2}\right)\right]^2 \qquad \text{Eq. 5-2}$$

$$b = \Omega_b \frac{RT_c}{P_c} \qquad \text{Eq. 5-3}$$

$$c = (1 - 3\zeta_c)\frac{RT_c}{P_c} \qquad \text{Eq. 5-4}$$

where Ω_b is the smallest positive root of the cubic,

$$\Omega_b^3 + (2 - 3\zeta_c)\Omega_b^2 + 3\zeta_c^2\Omega_b - \zeta_c^3 = 0 \qquad \text{Eq. 5-5}$$

$$\Omega_a = 3\zeta_c^2 + 3(1 - 2\zeta_c)\Omega_b + \Omega_b^2 + 1 - 3\zeta_c \qquad \text{Eq. 5-6}$$

where P is pressure, T is temperature, R is the universal gas constant, v is molar volume, T_c is the critical temperature, and P_c is the critical pressure. The pure component parameters F and ζ_c are fit to the vapor pressure data and molar volume of that component. All pure component data are shown in Table 5-1.

The Mathias-Klotz-Prausnitz (MKP) mixing rules with two binary interaction parameters, as shown in equations 5-7 to 5-8, was used for mixture calculations.

$$a = \sum_i x_i \sum_j x_j a_{ji}^{(0)}(1 - k_{ji}) + \sum_i x_i \left(\sum_j x_j \left(a_{ji}^{(0)} l_{ji}\right)^{1/3}\right)^3 \qquad \text{Eq. 5-7}$$

where, $$a_{ji}^{(0)} = \sqrt{a_i a_j} \qquad \text{Eq. 5-8}$$

A two parameter mixing rule was necessary to model the phase behavior in the non-ideal 2-propanol + carbon dioxide and the organic + water in this study studied. For multicomponent systems the use of two parameter models like those of Pagiotopolous

and Reid (Panagiotopolous and Reid 1986) with parameters regressed from binary data result in incorrect predictions. The MKP mixing rules are shown to be invariant for multicomponent mixtures (Mathias, Klotz et al. 1991). For all binary pairs, $k_{ij} = k_{ji}$ and $l_{ij} = -l_{ji}$, the following temperature dependency of the interaction parameters is used:

$$k_{ij} = k_{ij}^{(0)} + k_{ij}^{(1)} / T \qquad \text{Eq. 5-9}$$

$$l_{ij} = l_{ij}^{(0)} + l_{ij}^{(1)} / T \qquad \text{Eq. 5-10}$$

Linear mixing rules were used for parameters b and c, as shown in equations 5-11 and 5-12. The binary interaction parameters were found by minimizing the sum squared

$$b = \sum_i x_i b_i \qquad \text{Eq. 5-11}$$

$$c = \sum_i x_i c_i \qquad \text{Eq. 5-12}$$

deviation in pressure. The regressed interaction parameters are shown in Table 5-2.

For the method presented here the calculation proceeds as follows: the mole fraction of the liquid phase is first estimated from the liquid phase volume expansion and used to calculate the bubble pressure, vapor composition, and vapor molar volume. The experimental volume of the vapor phase is related to the total moles in the vapor phase by equation 5-13, where $V_{\exp}^{V}$ is the measured volume of the vapor phase, v_{EoS}^{V} is the calculated molar volume of the vapor phase, and n^{V} is the total number of moles in the vapor phase. The composition of the liquid phase is the difference in total moles of component i (n_i^{tot}) and the moles of component i in the vapor phase, as shown by

Table 5-1. Pure component parameters used in the Patel-Teja CEoS. Critical temperature and pressure from the DIPPR database. ζ_c and F calculated to match density and vapor pressure data taken from the DIPPR database.

Compound	T_c (K)	P_c (MPa)	ζ_c	F
Acetone	508.2	4.70	0.2819	0.7085
Argon	150.9	4.90	0.3280	0.4508
Carbon Dioxide	304.2	7.36	0.3106	0.7115
2-Propanol	508.3	4.76	0.3001	1.2814
Water	647.1	22.06	0.2690	0.6898

Table 5-2. Binary interaction parameters for the binary pairs for MKP with Patel-Teja EoS with references for data correlated.

Compound	$k_{ij}^{(0)}$	$k_{ij}^{(1)}$, K	$l_{ij}^{(0)}$	$l_{ij}^{(1)}$, K	*reference*
CO_2/2-Propanol	0.09769	5.42	0.26214	-67.83	[2]
CO_2/Argon	0.07	0	0	0	[5]
CO_2/Acetone	-0.1899	52.93	0	0	[2]
CO_2/Water	3.4288	-1158	-6.8546	2254	[1, 23]
2-Propanol/Argon	0.06	0	0	0	[14]
2-Propanol/Acetone	0.07973	-13.08	-0.1034	29.16	[18]
2-Propanol/Water	0.07728	-71.79	-0.2920	70.92	[19]
Argon/Acetone	0.06	0	0	0	[14]
Argon/Water	0.03	0	0	0	[3]
Acetone/Water	0.05077	-78.13	-0.1680	9.32	[13, 22]

equation 5-14. The mole fractions of the liquid phase input into the bubble pressure calculation are varied using a simplex algorithm until input and output mole fractions agree.

$$\frac{V_{\text{exp}}^{V}}{v_{\text{EoS}}^{V}} = n^{V} \qquad \text{Eq. 5-13}$$

$$n_i^{tot} - y_i^{\text{EoS}} n^{V} = n_i^{L} \qquad \text{Eq. 5-14}$$

Comparison to Literature Data

In order to verify the accuracy and dependability of gas loading and volume measurements in the experimental technique, the density of pure carbon dioxide and of a 4:1 carbon dioxide to argon mixture were measured at 313 K. As shown in Figure 5-4, the results for the density of pure carbon dioxide match the value as given by the Span-Wagner EoS for CO_2. The mixture of argon and carbon dioxide results in a mixture of lower density as expected and is predicted well by the Patel-Teja EoS.

The vapor-liquid equilibrium of the carbon dioxide + 2-propanol binary was measured at 313 K and compared to the literature data of Bamberger and Maurer which was measured by a flow technique (Bamberger and Maurer 2000). The data from this work are in good agreement, with slightly higher pressures for the high mole fractions of CO2 as shown in Figure 5-5. The Patel-Teja EoS with MKP mixing rules (PT-MKP) is able to fit the VLE well with the largest deviations present at mole fraction of CO_2 greater than 0.70.

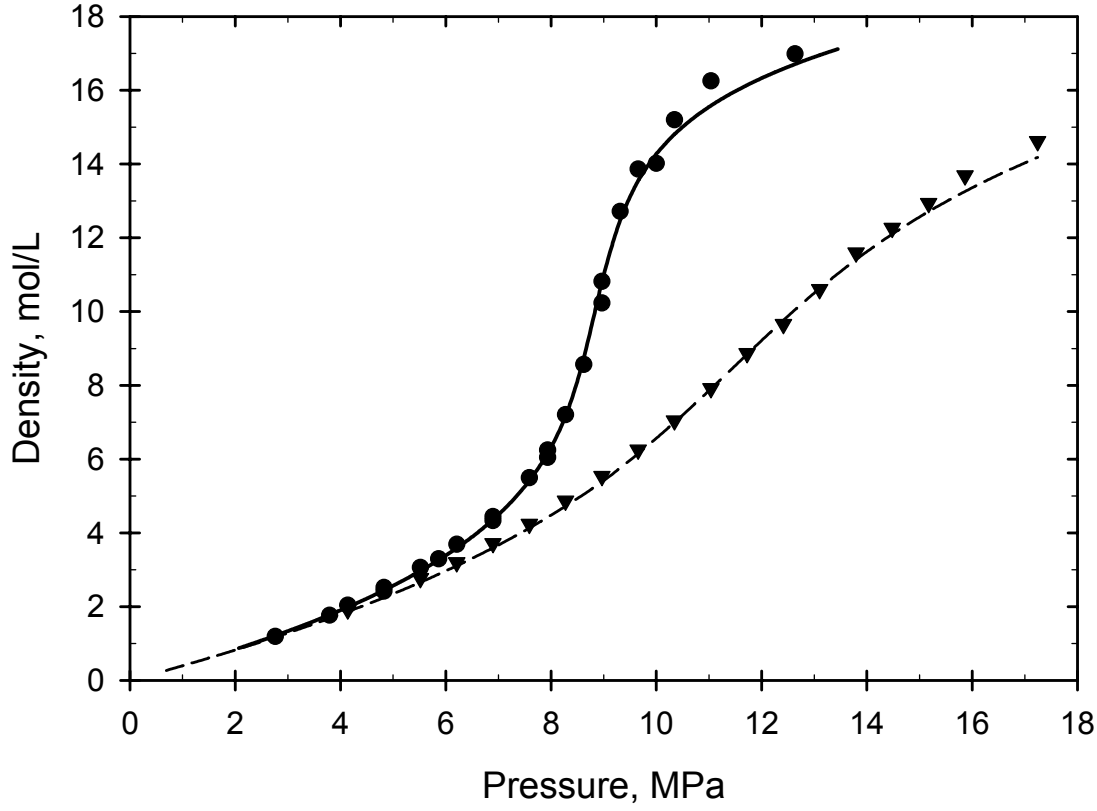

Figure 5-4. Density of CO_2 (▼)and CO_2 + Argon (80% CO_2, 20% Ar) mixture (●) as a function of pressure. Solid line Span-Wagner EoS. Hatched line Patel-Teja EoS.

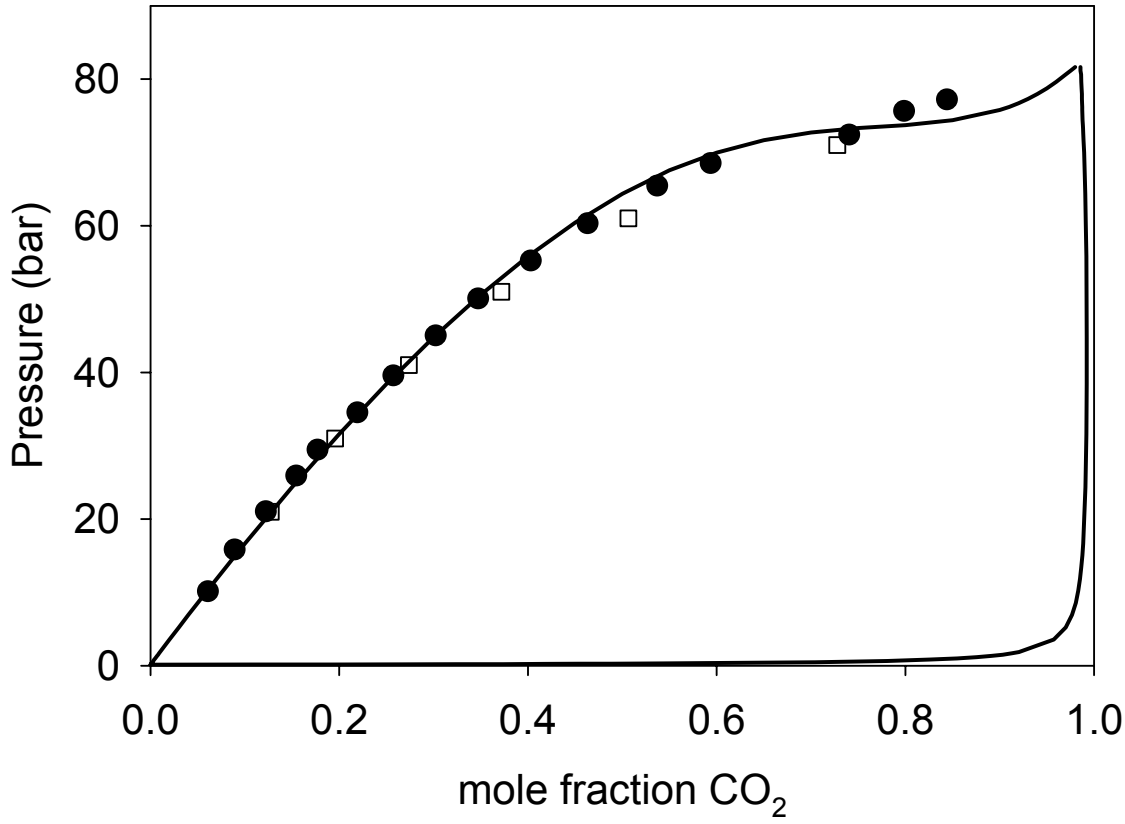

Figure 5-5. P-x-y diagram for system 2-Propanol/CO_2 at 313 K. (□) (Bamberger 2000) and (●) this work.

Experimental Results

The high-pressure vapor-liquid equilibria for the ternary system argon + carbon dioxide + 2-propanol was measured at 313 K and pressures of 6.9, 11.0, and 15.0 MPa. The results for the liquid phase compositions are shown in Table 5-3. As can be seen from Figure 5-6, the PT-MKP EoS is able to describe accurately the ternary phase behavior using only correlated binary interaction parameters.

At the lowest pressure of 6.9 MPa, we see as 2-propanol is replaced in the liquid phase with carbon dioxide the solubility of argon decreases to zero at the 2-propanol-CO_2 binary axis. This is required because at this pressure, we are below the critical pressure of the mixture and there exists a two phase region in the carbon dioxide + 2-propanol binary system. At concentrations of argon less than the equilibrium line a saturated liquid phase exists in equilibrium with a vapor phase with very low concentrations of 2-propanol. This liquid saturation line demonstrates the obvious preferential solubility of carbon dioxide over argon in 2-propanol.

At 11.0 MPa, which is above the binary critical pressure of the carbon dioxide + 2-propanol binary, CO2 and 2-propanol are miscible in all proportions. The increase in partial pressure of argon increases the argon solubility in the liquid phase. This no longer limits the single phase to the liquid-region, creating continuous single phase region that spans from the liquid region to a supercritical single phase region. At 15.0 MPa, with a further increase in partial pressure of argon, the solubility of argon in the liquid phase increases and the concentration range of the single phase region increases proportionally.

Table 5-3. Liquid phase composition in mole fraction of CO_2 (1) + 2-propanol (2) + argon (3) at 313 K and pressures of 6.9, 11.0 and 15.0 MPa.

T = 313 K, P = 6.9 MPa					
x_1	x_2	x_3	x_1	x_2	x_3
0.044	0.892	0.064	0.289	0.687	0.024
0.269	0.693	0.038	0.399	0.581	0.020
0.277	0.709	0.014	0.491	0.491	0.018
0.277	0.697	0.025			
T = 313 K, P = 11.0 MPa					
x_1	x_2	x_3	x_1	x_2	x_3
0.053	0.856	0.091	0.520	0.408	0.072
0.337	0.593	0.070	0.548	0.386	0.066
0.344	0.596	0.059	0.721	0.210	0.069
0.414	0.528	0.058	0.754	0.168	0.078
T = 313 K, P = 15.0 MPa					
x_1	x_2	x_3	x_1	x_2	x_3
0.061	0.814	0.125	0.438	0.458	0.104
0.363	0.548	0.089	0.460	0.437	0.103
0.372	0.514	0.114	0.566	0.314	0.121

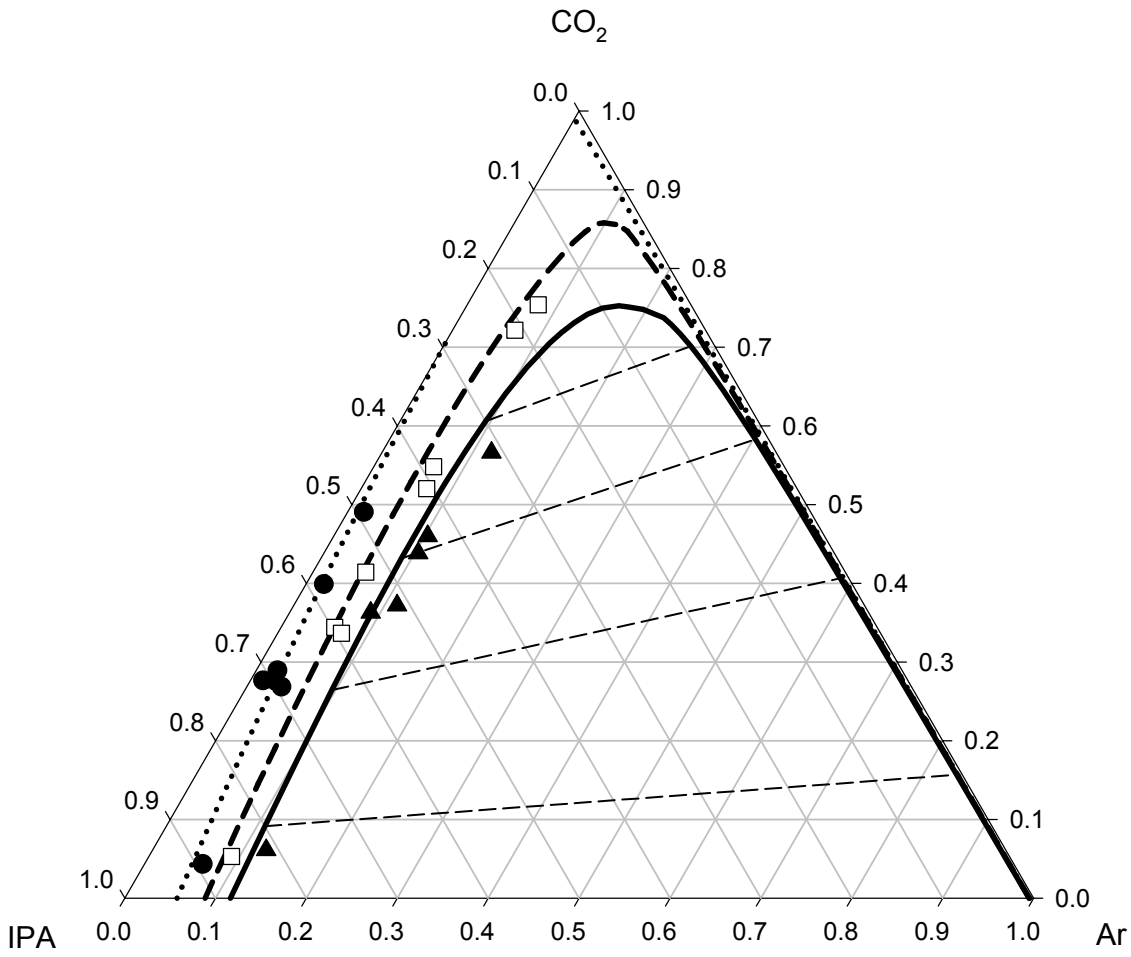

Figure 5-6. Vapor-liquid equilibria of carbon dioxide (CO_2) + argon (Ar) + 2-propanol (IPA) at 313 K and 6.9 MPa (●), 11.0 MPa (□), and 15.0 MPa (▲). Lines are Patel-Teja EoS with hatched tie-lines represent equilibrium concentrations of liquid and vapor at 15.0 MPa.

The predicted tie-lines are shown for the liquid phase in equilibrium with the vapor phase.

At 11.0 and 15.0 MPa there is a minimum in argon solubility versus the ratio of carbon dioxide to 2-propanol in the liquid phase. At isobaric conditions, as carbon dioxide is added to the system the partial pressure of argon is decreased thus tending to decrease the solubility in the liquid phase (there is less argon present). In addition, of opposite effect is the enhanced solubility of argon in carbon dioxide versus that of 2-propanol (H_{CO2} = 43.0 MPa , H_{ISOP} = 84.7 MPa). The decrease in the partial pressure of argon dominates for low CO_2 concentrations, but as more CO_2 replaces 2-propanol the enhanced solubility dominates and the solubility begins to increase. This balance of enhanced solubility and the dilution effect of carbon dioxide can be considered in terms of the ratio of reactants in solution which we know is an important factor in the rate of reaction. The ratio of argon to 2-propanol increases for higher ratios of carbon dioxide to 2-propanol, and at higher pressures the effect is more pronounced, as shown in Figure 5-7. So that while the solubility of argon may not always be increased with CO_2 it seems the ratio of reactants can be increased at pressures above the CO_2 + 2-propanol two phase region.

The effect of product formation on the phase equilibria was also considered. The phase equilibria of carbon dioxide + argon + 2-propanol + acetone + water was measured along the reaction coordinate by constructing synthetic reaction mixtures at degrees of 2-propanol conversion. Three pressures were investigated (6.9, 11.0, and 15.0 MPa) at a temperature of 313 K. A process was idealized as premixed gas feed and liquid reactant

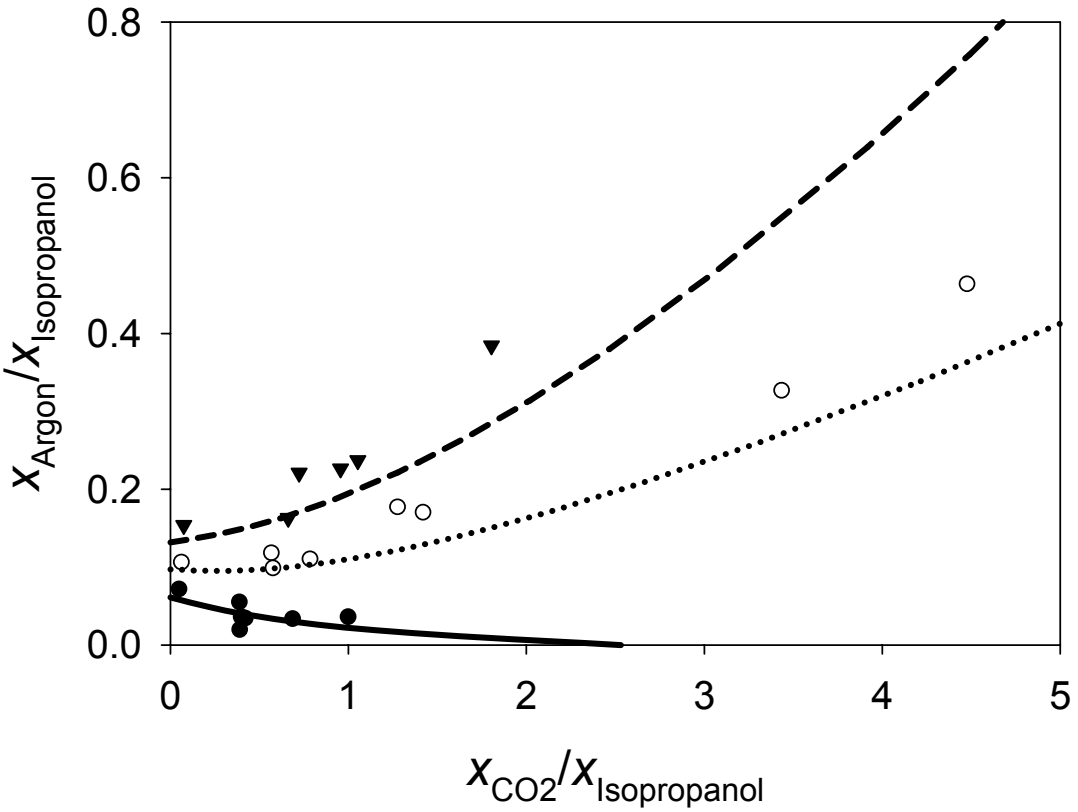

Figure 5-7. Change in the ratio of reactants in the liquid phase versus dilution of 2-propanol with carbon dioxide in the liquid phase at 313 K and 6.9 MPa (●), 11.0 MPa (○), and 15.0 MPa (▼).

feed to a continuously stirred tank reactor (CSTR). The argon was assumed to be in excess with the overall molar ratio of carbon dioxide to argon maintained at 3:1. The dilution of the liquid phase was maintained at a carbon dioxide to (2-propanol + acetone + water) molar ratio of 3:4. The change in mole fraction solubility of argon in the liquid phase as a result of conversion of 2-propanol is shown in Figure 5-8.

The reaction products decrease the solubility of argon in the liquid phase up to a 2-propanol conversion of 33% and appear to level out or possibly increase at higher conversions. There are two main competing effects in this mixture. The increasing presence of water in the system lowers the solubility of argon. However, the presence of acetone increases the solubility of carbon dioxide in the liquid phase and thus enhances the solubility of argon. At high enough conversions (water concentrations) and pressures a second liquid phase is present. The concentrations of the 3-phase system (V-L-L) is not obtainable using this technique, however the second liquid phase is most likely a water-rich phase in equilibrium with two carbon dioxide rich phases, the other liquid and the vapor phase.

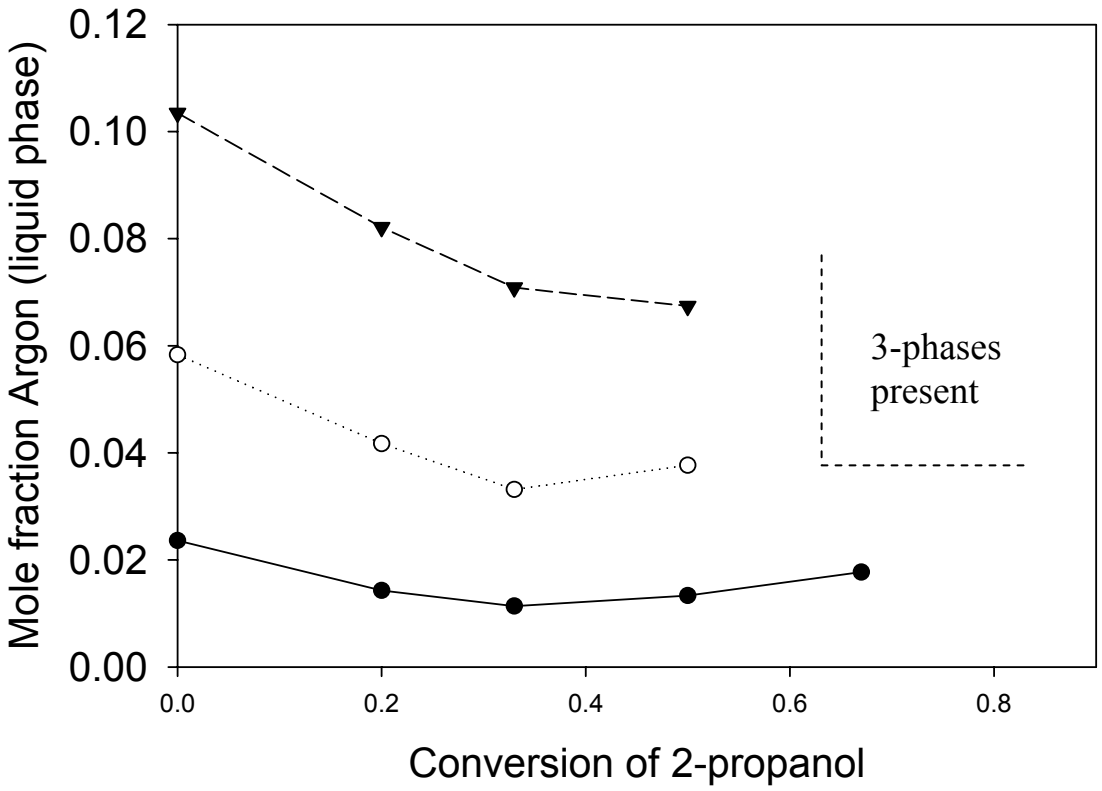

Figure 5-8. Mole fraction of Argon in the liquid phase vs. conversion of 2-propanol to acetone and water at 313 K and 6.9 MPa (●), 11.0 MPa (○), and 15.0 MPa (▼).

Summary

The solubility of argon in mixtures of carbon dioxide and 2-propanol were measured at 313 K and from 6.9 to 15.0 MPa. We believe that the behavior of oxygen in this solution will not be substantially different, and the results found here applicable to oxygen. The high-pressure phase VLE was found to be predicted well by the Patel-Teja EoS using only interaction parameters regressed from binary data. With increasing pressure the two phase region was found to decrease in size. The mole fraction solubility of argon in the liquid phase was observed to go through a minimum due to the opposing effects of dilution and enhanced solubility that carbon dioxide contributes to the system.

The effect of product formation on the phase equilibria was also considered. The mole fraction solubility of argon in synthesized mixtures of CO_2 + 2-propanol + acetone + water was measured at 313 K and 6.9 to 15.0 MPa. The solubility was found to decrease and then level out as more product is added to the system. At high pressures and high concentrations of product the formation of a second liquid phase is possible.

Nomenclature

a = equation of state attractive parameter
b = equation of state volume parameter
c = equation of state volume parameter
F = pure component equation of state parameter
k = binary interaction parameter
l = binary interaction parameter
n = number of moles
P = pressure
R = universal gas constant
T = temperature
v = molar volume
V = volume
x = mole fraction

Greek

ζ_c = pure component equation of state parameter
Ω_a = equation of state parameter
Ω_b = equation of state parameter

Superscripts and Subscripts

c = critical point value
EoS = calculated from an equation of state
exp = experimentally determined
i,j = component indices
L = liquid phase value
tot = total (sum of liquid and vapor phases)
V = vapor phase value

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CHAPTER VI

HIGH PRESSURE PHASE EQUILIBRIA OF SOME CARBON DIOXIDE + ORGANIC + WATER SYSTEMS

Introduction

Supercritical carbon dioxide, although an inert diluent, can increase rates and/or selectivity for both homogeneous and heterogeneous catalyzed reactions and improve recovery of homogenous catalysts (Musie, Wei et al. 2001; Tschan, Wandeler et al. 2001; Ablan, Hallett et al. 2003). For reactions that involve permanent gases (e.g. O_2, CO, and H_2) and liquids, the addition of carbon dioxide can improve the mutual solubility (Gläser, Williardt et al. 2003) (Bezanehtak, Dehghani et al. 2004; Xie, Brown et al. 2004) and lower resistance to mass transfer. (Sassiat, Mourier et al. 1987)

In homogeneous catalysis, we take advantage of the unique phase behavior of carbon dioxide. CO_2 is the only nontoxic, nonflammable solvent that is miscible with fluorocarbons, hydrocarbons, and most low molecular weight polar organics like alcohols, ethers, ketones, nitriles, and nitroalkanes, but it is immiscible with water. For fluorous-organic biphasic solvent systems (Horváth and Rábai 1994), CO_2 can be added to run these reactions homogeneously with improved reaction rates (West, Hallett et al. 2003). CO_2 can also be used to improve water-organic biphasic solvent systems. The

traditional water/organic biphasic technique, popularized by the Ruhrchemie/Rhône-Poulenc process (Kohlpainter, Fischer et al. 2001) requires a water-insoluble solvent, which is required to recycle the hydrophilic catalyst. The use of a water-insoluble solvent will obviously create a biphasic system which can hinder mass transfer of reactants across the interface (Watchsen, Himmler et al. 1998). Here the addition of a polar organic co-solvent creates the opportunity to run homogeneous reactions in an organic/aqueous mixture with a hydrophilic catalyst. The solubility of hydrophobic reactants, such as long chain olefins, can be made miscible by the addition of the organic co-solvent. The dissolution of gaseous carbon dioxide into the water/tetrahydrofuran mixture will cause the formation of two liquid phases. The catalyst-rich aqueous phase and the product-rich organic phase can be easily decanted and the aqueous catalyst recycled.

Traditional organometallic ligands, such as triphenyl phosphine (PPh_3) have been modified via sodium sulfonate attachments on the aromatic rings to make them water soluble. This charged species, triphenylphosphinetrisulfonate (TPPTS) has preferential solubility in the water layer of any aqueous biphasic mixture. Investigations into the partitioning of water soluble dyes similar to the mentioned ligands, like the chromatotrope FB dye shown in Figure 6-1A, have shown preferential partitioning into the water phase of 67000:1 (Lu, Lazzaroni et al. 2004). An example of an actual catalyst used for hydroformylation reactions, as shown in Figure 6-1C, should partition even better given the presence of the additional sulfonate groups.

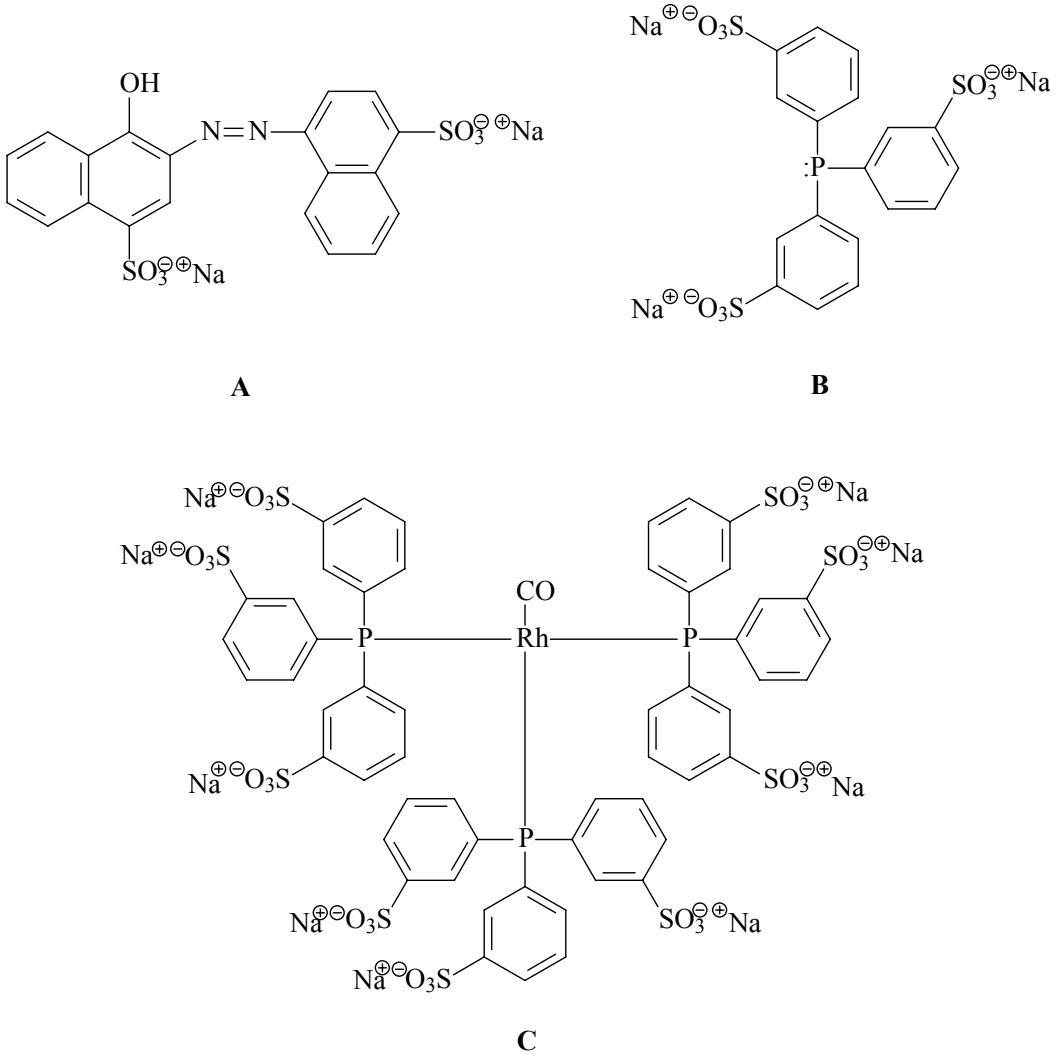

Figure 6-1. Structures of the water-soluble compounds. **A** – The dye chromatotrope FB. **B** – The ligand TPPTS. **C** – A rhodium-based hydroformylation catalyst (Herrmann 1993).

Extensive work has been done examining the solubility of carbon dioxide in organic liquids, creating "gas-expanded liquids" and several comprehensive reviews summarizing the currently available data are available (Christov and Dohrn 2002). Because carbon dioxide is miscible with many organic solvents but immiscible with water, it is of particular interest in separating the organic solvent from an aqueous mixture and thus sequestering a water soluble catalyst. This difference in solubility allows the use of water-miscible organics and extends the concept of water/organic biphasic solvent systems.

Francis (Francis 1954) was the first to examine extensively ternary systems containing carbon dioxide. He reported 464 phase diagrams in qualitative form for liquid CO_2 and various combinations of two liquid phases (mostly aqueous/organic or organic/organic.) Many of these liquids were not pure, but industrial oil mixtures that were conveniently available. Recent investigators have examined some carbon dioxide + organic + water phase behavior, specifically examining systems with the organic component as alcohols (Wendland, Hasse et al. 1993), ketones (Traub and Stephan 1990) and some other systems (Briones, Mullins et al. 1987; Lee, Reighard et al. 1996). There is little data available for systems involving liquid-liquid equilibria of more polar, aprotic organic solvents with water and carbon dioxide.

To investigate the feasibility of these processes, vapor-liquid-liquid phase equilibria in mixtures of water + CO_2 + tetrahydrofuran, 1,4-dioxane, or acetonitrile were studied at 298, 313, and 333 K and pressures ranging from 1.0 to 5.7 MPa. In addition,

the water-organic partition coefficients of 1-octene, a potential reactant of interest, was measured as a function of applied CO_2 pressure.

To correctly describe the pressure effect on the liquid-liquid equilibria of these systems, especially since they involve a supercritical component, an equation of state is necessary to quantitatively describe the phase behavior. The organic + water systems investigated in this work are difficult to correlate with cubic equations of state using traditional mixing rules, i.e. van der Waals. More recent mixing rule models that match the excess free energies from the equation of state with that of an independent activity coefficient model have been shown to be successful at correlating the VLE of carbon dioxide + organic systems (Orbey and Sandler 1997) and the LLE of oxygenated alkanes + water systems (Escobedo-Alvarado and Sandler 1998). In this work, the Peng-Robinson cubic equation of state (Peng and Robinson 1976) with the modification of Stryjek and Vera (Stryjek and Vera 1986) is used along with the several modifications of the Huron-Vidal mixing rules.

Experimental Materials

HPLC grade tetrahydrofuran (99%), 1,4 dioxane (99%), acetonitrile (99%), water (99%) , and 1-octene (98%) were obtained from Aldrich Chemical Co. and were used as received. SFC Grade carbon dioxide (99.99%) was obtained from Matheson Gas Products. The CO_2 was further purified to remove trace water using a Matheson (Model 450B) gas purifier and filter cartridge (Type 451).

Apparatus and Procedure

VLLE Apparatus

Figure 6-2 shows a schematic of the equilibrium cell apparatus. The equilibrium cell consists of a hollow sapphire cylinder (50.8 mm O.D. × 25.4±0.0001 mm I.D. × 203.2 mm L) with a movable stainless steel piston inside and stainless steel end caps. The cell is divided into two chambers separated by an o-ring seal on the piston, one side containing the equilibrium components and the other side containing the pressuring fluid, in this case water. The equilibrium cell was placed in a temperature controlled air bath. The temperatures of the air bath and vapor phase inside the cell were monitored with thermocouples (Omega Type K) and digital readouts (HH-22 Omega). The air bath temperature was maintained by a digital temperature controller (Omega CN76000) with an over temperature controller (Omega CN375) for safe operation. The temperature was accurate to within ±0.2 K and calibrated against a platinum RTD (Omega PRP-4) with a DP251 Precision RTD Benchtop Thermometer (DP251 Omega) accurate to ±0.025 K and traceable to NIST. The pressures were measured with a pressure transducer and digital read-out (Druck, DPI 260, PDCR 910). The transducer was calibrated against a hydraulic piston pressure gauge (Ruska) to an uncertainty of ± 0.01 MPa. The liquid phase compounds are added to the cell using a gas-tight syringe. The syringe was weighed before and after liquid addition to find mass added and had an estimated error of less than ±0.05 grams or less than ±0.1% of mass loaded. CO_2 was added to the cell from a syringe pump (ISCO, Inc., Model 500D) operated at a constant pressure and temperature. Using the volume displacement of the syringe and the highly accurate Span-Wagner EOS

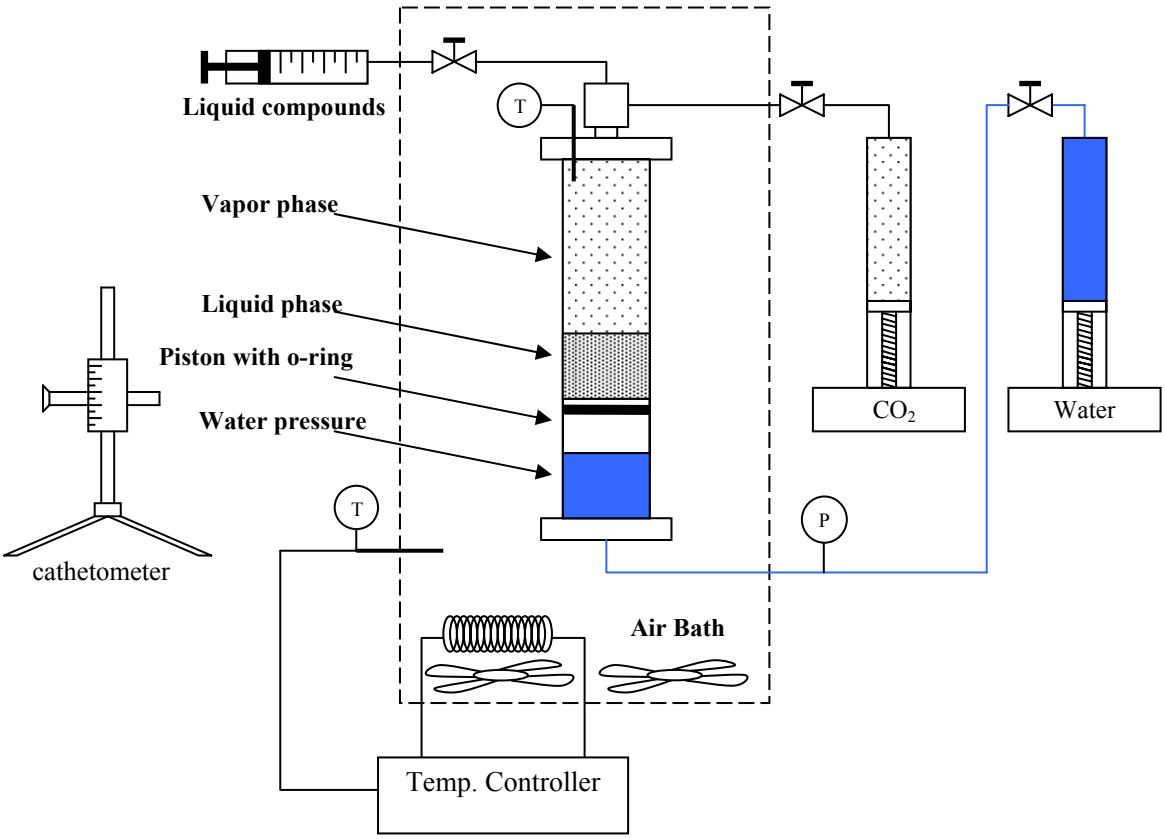

Figure 6-2. Schematic of equilibrium cell apparatus.

(Span and Wagner 1996), the moles of CO_2 added to the cell is calculated with an error of ± 0.001 moles, or for the smallest loading an error of ±1.5% in moles added. Liquid and vapor volumes are calculated by measuring the height of the meniscus with a micrometer cathetometer. For displacements less than 50 mm, the accuracy is 0.01 mm; for larger displacements, the accuracy is 0.1 mm. The cell is mounted on a rotating shaft, and mixing is achieved by rotating the entire cell.

VLLE Experimental Procedure.

The procedure followed for measuring the phase equilibria of the ternary system is the synthetic technique similar to that of Laugier, et al. (Laugier, Richon et al. 1990) and DiAndreth, et al. (DiAndreth, Ritter et al. 1987) The technique uses visual data collected from multiple loadings to solve a set of material balances for composition rather than directly sampling the equilibrium phases. This technique and other synthetic techniques avoid the inherent errors and difficulties in direct sampling. Direct sampling from high pressure systems pose potential problems with phase separation or flashing caused by changes in pressure or temperature in the sample line.

Equations 6-1, 6-2 and 6-3 represent the overall material balance and two of the component material balances for a three-phase, three-component system. The third component balance is linearly dependent on these three equations. N represents the number of moles, V the volume of a phase α, β or ν, $\boldsymbol{\nu}$ the molar volume, and $\boldsymbol{x}_i$ the mole fraction of component i in phase α, β or ν.

$$N_T = \frac{V^\alpha}{\nu^\alpha} + \frac{V^\beta}{\nu^\beta} + \frac{V^v}{\nu^v} \qquad \text{Eq. 6-1}$$

$$N_1 = \frac{x_1^\alpha V^\alpha}{\nu^\alpha} + \frac{x_1^\beta V^\beta}{\nu^\beta} + \frac{x_1^v V^v}{\nu^v} \qquad \text{Eq. 6-2}$$

$$N_2 = \frac{x_2^\alpha V^\alpha}{\nu^\alpha} + \frac{x_2^\beta V^\beta}{\nu^\beta} + \frac{x_2^v V^v}{\nu^v} \qquad \text{Eq. 6-3}$$

In this method, the number of moles (N_1, N_2, N_T) would be known from loading the cell, and the volumes are measured at given conditions via the method previously described using the cathetometer. This leaves the mole fractions (x_1^α, x_1^β, x_1^v, x_2^α, x_2^β and x_2^v) and molar volumes (ν^α, ν^β, ν^V) as unknown variables. Since there are nine variables and only three equations, the system cannot be solved. However, using three loadings at the same temperature and pressure, six additional balances are available, without any added unknowns. This is because the mole fractions and molar volumes are state variables that are defined for a given temperature and pressure and are independent of overall composition, as long as there are three components and three phases. With the second and third loadings, there are now nine independent equations that can be solved for the nine variables. In this experiment, five loadings were performed for greater precision and to eliminate the dependence of the result upon each loadings measurement. Care does have to be taken in making each loading contribute to the calculation of the composition. The volume ratio of the two liquid phases must vary or the analysis will

result in some dependent equations and yield unreliable results. By loading different volume ratios of the liquid components this can be avoided.

Additionally, the composition and molar volume of the vapor phase were assumed from known data. Since one of the liquid phases is mostly water, the partial pressure of water in the vapor phase was assumed to be the vapor pressure, and the composition of the other two components was predicted from correlated binary data. The molar volume of the vapor phase was assumed to be that of pure CO_2, since the composition is never less than 98% CO_2.

Partitioning Apparatus

The distribution coefficients were measured in a windowed 316 stainless steel stirred autoclave (Parr model 4780) with an internal volume of 350 ml. The vessel was heated by a thermostatted heating jacket. Agitation in the vessel was maintained at 200 ± 5 rpm using a four-blade 85^{o} pitched-blade impeller. A PID temperature controller and tachometer (Parr Instrument Company, Model 4842) were used to control the temperature of the reactor to ± 1 K and the stirring speed to ± 5 rpm. The temperature inside the reactor was monitored with a type J thermocouple (Omega) and the pressure with a digital pressure transducer (Heise, Model 901B). Two six-port valves and sample loops (Valco Instruments Co. Inc.) with various volumes were used to take samples from each of the two phases in the reactor. Each valve was attached to a dip tube; one reaching to the vessel bottom and the other approximately 2 cm above the liquid-liquid meniscus. The sample loop volumes were calibrated to ±2%.

Partitioning Experimental Procedure

Measurement of the distribution coefficients of 1-octene were performed at 25 ºC. Degassed tetrahydrofuran (35 mL), water (15 mL), and 1-octene (1 mL) were loaded into the windowed Parr vessel, which was then sealed. CO_2 was then added from a syringe pump (ISCO, Inc., Model 500D). The vessel was then heated and stirred to equilibrium and the pressure recorded. The stirring was discontinued during sampling. The sample loop was flushed with approximately three times its volume of the phase being sampled, then the valve position was switched and the sample loop was emptied and flushed with at least six times its volume of tetrahydrofuran. This procedure was performed on samples from each liquid phase. The concentrations of 1-octene in each phase was determined using an Agilent 6890 gas chromatograph equipped with a flame ionization detector and the response was calibrated using standards of known concentration.

Experimental Results

The high-pressure vapor–liquid–liquid equilibria of carbon dioxide + tetrahydrofuran (THF) + water were measured at 298 K, 313 K, and 333 K and at pressures from 1.0 to 5.2 MPa. Composition and molar volume results are shown in Table 6-1. The composition of the vapor phase is not shown in the tables nor in Figures 6-7 to 6-11.

To verify the synthetic technique, the top organic rich phase was sampled with a technique similar to that described in Chapter VII. The samples were analyzed using GC-FID. The samples were taken at 4 pressures, 1.03, 1.55, 2.07, and 3.10 MPa,

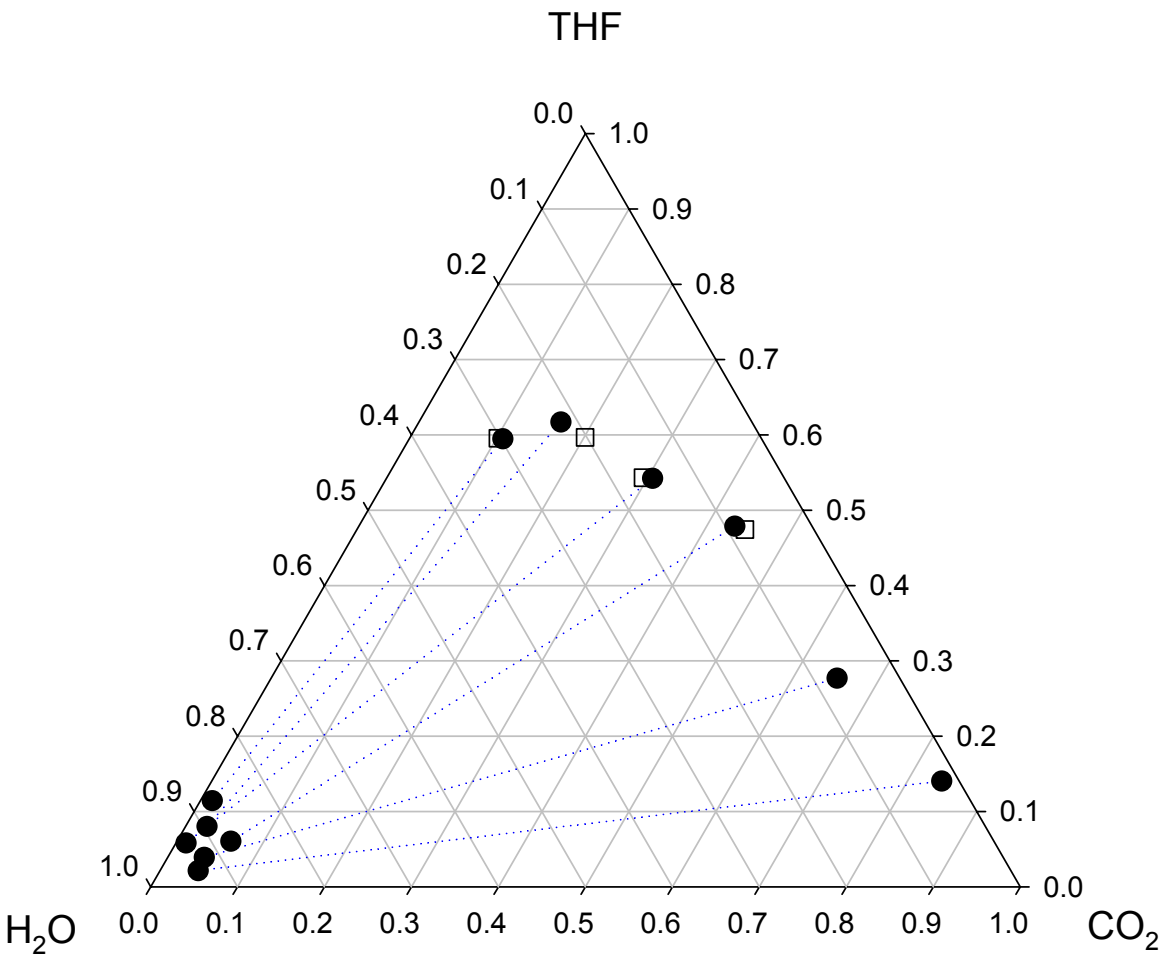

Figure 6-3. Comparison of experimental methods. (●) Synthetic method, (□) Analytical method

Table 6-1. LLE of Carbon Dioxide + Tetrahydrofuran + Water System at 298, 313, and 333 K.

		Liquid phase 1 (L_1)				Liquid phase 2 (L_2)				Vapor
T (K)	P (MPa)	x_{CO2}	x_{THF}	x_{H2O}	v_L (cm^3/mol)	x_{CO2}	x_{THF}	x_{H2O}	v_L (cm^3/mol)	v_V (cm^3/mol)
298	1.03	0.014	0.114	0.872	23.7	0.107	0.595	0.298	55.5	2269.1
298	1.55	0.025	0.080	0.895	21.8	0.163	0.617	0.220	61.0	1467.6
298	2.07	0.012	0.058	0.930	20.2	0.306	0.542	0.152	58.9	1065.2
298	3.10	0.062	0.060	0.878	18.7	0.432	0.479	0.089	79.8	658.8
298	4.14	0.042	0.039	0.919	19.4	0.651	0.277	0.072	54.1	449.4
298	5.17	0.044	0.021	0.935	18.1	0.839	0.140	0.021	53.3	316.0
313	0.99	0.013	0.117	0.870	25.1	0.045	0.511	0.444	53.4	2512.6
313	2.42	0.028	0.072	0.900	21.7	0.230	0.545	0.225	62.0	957.9
313	3.86	0.015	0.047	0.938	20.2	0.421	0.464	0.115	60.0	549.5
313	4.49	0.005	0.038	0.957	20.7	0.557	0.381	0.062	58.0	451.9
313	5.21	0.030	0.033	0.937	19.9	0.625	0.324	0.051	59.1	367.4
333	1.03	0.002	0.102	0.896	24.0	0.055	0.535	0.410	58.0	2581.3
333	2.07	0.006	0.064	0.930	22.3	0.116	0.559	0.325	55.5	1240.7
333	3.10	0.003	0.042	0.955	21.0	0.225	0.573	0.202	59.2	791.1
333	4.14	0.021	0.040	0.939	20.5	0.308	0.546	0.146	64.6	565.3
333	5.17	0.018	0.025	0.957	20.4	0.407	0.454	0.139	58.0	428.6

corresponding with the first points of the synthetic technique. As can be seen in Figure 6-3, there is excellent agreement between the synthetically determined data and the sampled data, thus confirming the accuracy and reliability of the synthetic data.

The addition of carbon dioxide to the miscible binary of tetrahydrofuran + water resulted in the formation of a water rich phase (>90 mole% for pressures > 2.0 MPa), with a nearly constant amount of carbon dioxide present and a carbon dioxide + organic rich phase where the carbon dioxide amount increases with increasing pressure. The LLE behavior of the carbon dioxide + tetrahydrofuran + water system was of interest because of the known closed loop critical behavior of the tetrahydrofuran + water binary system (Matous, Novak et al. 1972). The temperature at which tetrahydrofuran and water will form two liquid phases can be significantly lowered by introduction of modest amounts of carbon dioxide pressure, as can be seen in Figure 6-4. The two phases can be made purer (relative to the amount of water and tetrahydrofuran) by the addition of more carbon dioxide pressure. The small amount of tetrahydrofuran in the water-rich phase causes the error in the THF content in the water rich phase to be high. This plot demonstrates some of the competing effects present in this system; at 298 K there is more carbon dioxide present in both phases than at higher temperatures, causing a better phase split. At higher temperatures there is less carbon dioxide present, but the THF and water are approaching the lower critical solution temperature (LCST) for the pure binary allowing for a better phase split.

We attempted to measure the LLE at sub-ambient temperatures and found the appearance of a solid phase. Tetrahydrofuran and water mixtures are known to form

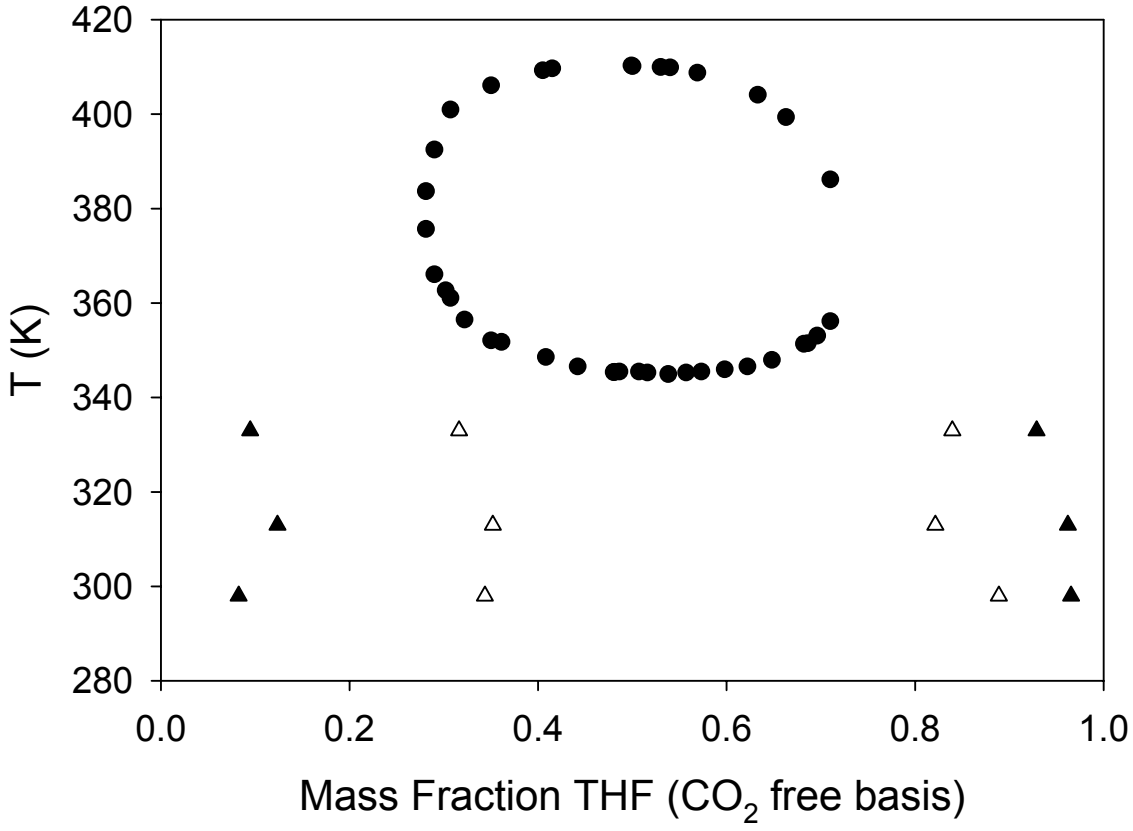

Figure 6-4. LLE for pure THF + H_2O and for CO_2 + THF + H_2O normalized to a CO_2 free basis. (●),(Matous, Novak et al. 1972); (△) 1.0 MPa CO_2 and (▲) 5.2 MPa CO_2, this work

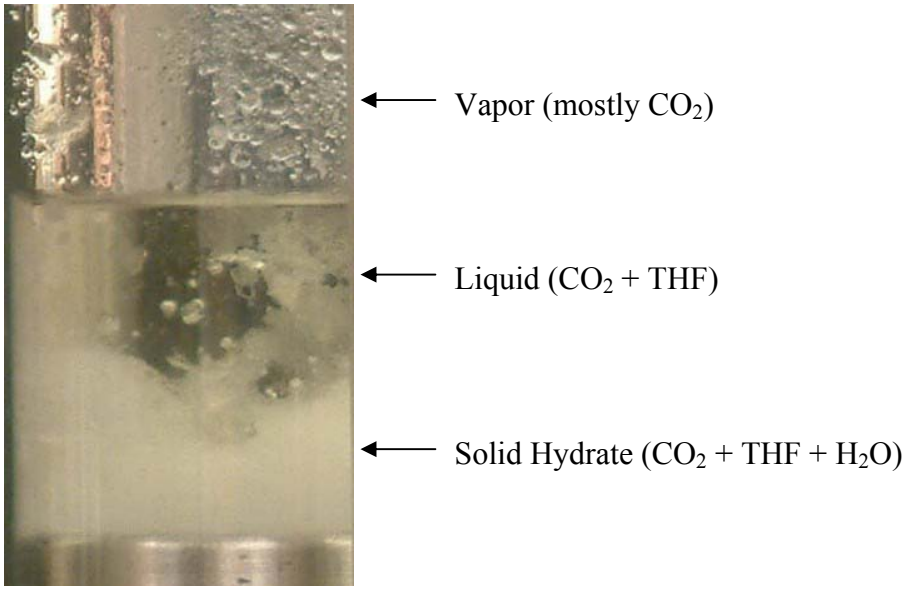

Figure 6-5. Picture of SLE of CO_2-THF-water system at 288 K and 3.0 MPa.

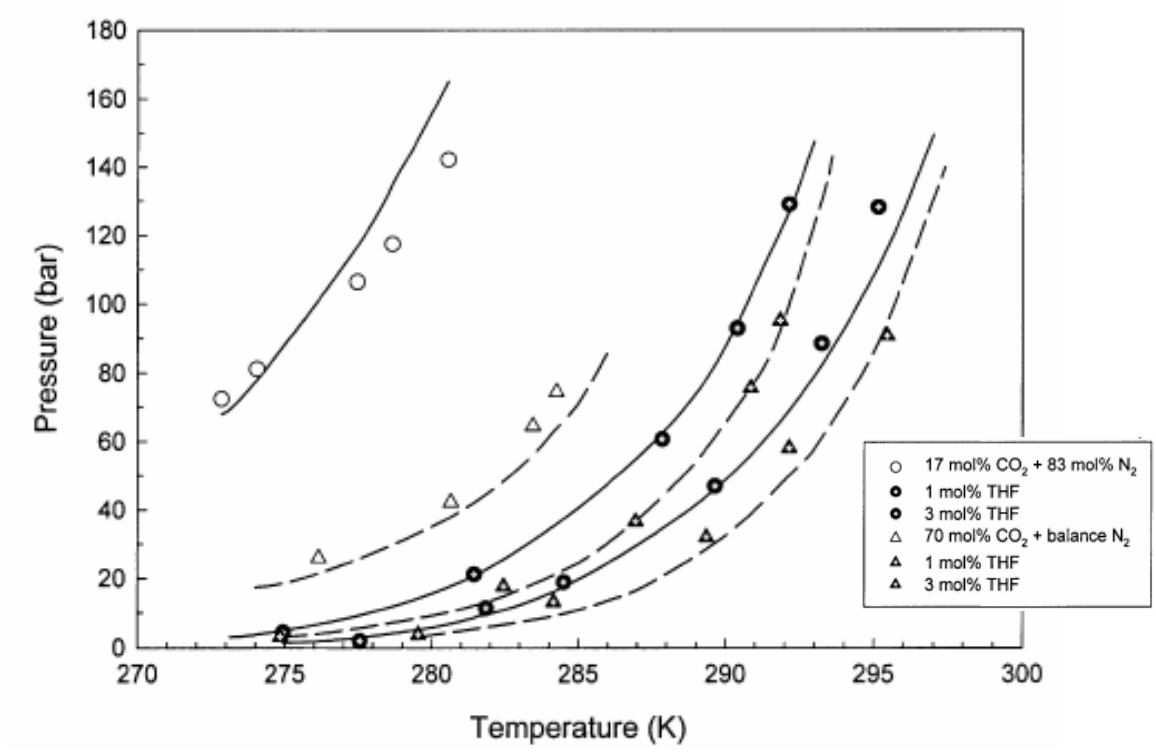

Figure 6-6. P-T relationship for formation of hydrates in the tetrahydrofuran + water system with various mixtures of CO_2 and N_2. Plot used from Kang, et al. (2001)

clathrate-hydrates, and the temperature at which the solid hydrates form can be raised by the addition of carbon dioxide which acts as a "help gas" (Sloan 1990). At 288 K with 3.0 MPa of carbon dioxide added, the denser water rich phase transitioned from the liquid phase to a solid, presumably a hydrate. A picture of the solid hydrate-liquid-vapor equilibrium is shown in Figure 6-5. This is consistent with the available literature data of Kang (Kang, H.Lee et al. 2001), who measured the clathrate hydrate phase equilibria of tetrahydrofuran + water under pressure of various mixtures of carbon dioxide and nitrogen. As shown in Figure 6-6, the appearance of clathrate-hydrates is possible at ambient temperatures (298K) with 15 MPa of carbon dioxide pressure. It should not be necessary to operate at a pressure this high to efficiently partition a catalyst, as a very pure water phase and organic phase are achieved at pressures around 5 MPa.

The high-pressure vapor–liquid–liquid equilibria of carbon dioxide + acetonitrile (ACN) + water were measured at 313 K and at pressures from 1.9 to 5.2 MPa. Composition and molar volume are shown in Table 6-2. The carbon dioxide + acetonitrile + water system required very little carbon dioxide pressure to cause a phase split similar to that of the tetrahydrofuran-ternary system, however the water rich phase contained more of the organic component (acetonitrile) than in the tetrahydrofuran system.

The high-pressure vapor–liquid–liquid equilibria of carbon dioxide + 1,4-dioxane (DIOX) + water were measured at 313 K and at pressures from 2.8 to 5.7 MPa. Composition and molar volume are shown in Table 6-3. The pressure required to cause a

Table 6-2. LLE of Carbon Dioxide + Acetonitrile + Water System at 313 K.

		Liquid phase 1 (L_1)				Liquid phase 2 (L_2)				Vapor
T (K)	P(MPa)	x_{CO2}	x_{ACN}	x_{H2O}	v_L (cm^3/mol)	x_{CO2}	x_{ACN}	x_{H2O}	v_L (cm^3/mol)	v_V (cm^3/mol)
313	1.9	0.038	0.229	0.733	25.7	0.076	0.435	0.489	33.6	1283.7
313	2.4	0.019	0.136	0.845	21.0	0.170	0.594	0.237	42.7	960.6
313	3.1	0.010	0.067	0.924	20.1	0.258	0.624	0.119	44.1	717.9
313	4.1	0.011	0.082	0.907	18.0	0.407	0.527	0.066	49.7	503.0
313	5.2	0.025	0.056	0.918	18.7	0.495	0.434	0.071	46.6	370.9

Table 6-3. LLE of Carbon Dioxide + 1,4-Dioxane + Water System at 313 K.

		Liquid phase 1 (L_1)				Liquid phase 2 (L_2)				Vapor
T (K)	P (MPa)	x_{CO2}	x_{DIOX}	x_{H2O}	v_L (cm^3/mol)	x_{CO2}	x_{DIOX}	x_{H2O}	v_L (cm^3/mol)	v_V (cm^3/mol)
313	2.8	0.081	0.247	0.672	35.0	0.200	0.435	0.365	52.8	819.7
313	2.9	0.055	0.210	0.735	32.8	0.247	0.434	0.319	49.8	768.0
313	3.1	0.037	0.174	0.789	29.8	0.309	0.458	0.233	53.2	717.9
313	3.8	0.018	0.115	0.867	24.5	0.443	0.433	0.125	57.6	562.1
313	4.3	0.025	0.091	0.884	22.9	0.509	0.374	0.117	55.8	471.9
313	4.8	0.031	0.062	0.907	21.6	0.573	0.350	0.077	56.8	409.2
313	5.7	0.013	0.047	0.940	19.3	0.709	0.262	0.029	56.0	321.3

liquid-liquid phase split was higher than the tetrahydrofuran-ternary system and resulted in a less pure water-rich phase and more water in the dioxane-rich phase.

The difference in phase behavior can be explained by considering the intermolecular interactions of these systems. If we consider the liquid-liquid phase behavior as the partitioning of the organic between a carbon dioxide rich phase and a water rich phase, the interactions and phase behavior can be elucidated. There is some difference in the VLE for carbon dioxide with any of the three organics, with carbon dioxide + acetonitrile showing small positive deviations from ideality, however they are essentially ideal $\gamma^{\infty} \approx 1$ and are not as differentiating when compared to the dominating effect of the water + organic behavior. For the organic and water interactions the infinite dilution activity coefficients $\left(\gamma^{\infty}\right)$ of the three organics in water at 298 K offers a basis of comparison and as measured by Dallas and co-workers (Sherman, Trampe et al. 1996) are as follows: $\gamma^{\infty}_{THF} = 17.01$, $\gamma^{\infty}_{ACN} = 11.10$, and $\gamma^{\infty}_{DIOX} = 5.42$. It is clear that the tetrahydrofuran + water system deviates furthest from ideality and therefore would be expected to be the most susceptible to phase splitting with the addition of a hydrophobic/organophilic component. The more ideal mixture of dioxane and water can be attributed to the additional basic ether functionality of 1,4-dioxane. This allows 1,4-dioxane to be solvated to a greater extent by the hydrogen bonded network present in a water solution than the single ether tetrahydrofuran. Because of the more favorable interactions of 1,4-dioxane with water, we expect to see and have experimental confirmation that both equilibrium phases are less pure (more water in the organic phase, more organic in the aqueous phase).

Acetonitrile is more polar than tetrahydrofuran, with a Kamlet-Taft π^* of 0.75 versus 0.58 for tetrahydrofuran, and thus has more favorable interactions with water due to stronger dipole-dipole interactions. Thus, the aqueous phase contains more organic component than the comparable phase in the tetrahydrofuran system, while the organic rich phase possesses similar amounts of water.

The infinitely dilute partitioning of 1-octene between the water rich and organic rich phase was measured as a function of added carbon dioxide in the carbon dioxide + tetrahydrofuran + water ternary system. The results are shown in Table 6-4. At low pressures the concentration of 1-octene is 10 times greater in the tetrahydrofuran-rich than the water-rich phase and increases to 3000 times greater at a pressure of 1.7 MPa. The addition of small amounts of carbon dioxide causes a large change in water content in the two equilibrium phases. As the pressure is increased the activity of 1-octene in the water rich phase greatly increases with less change in the organic rich phase, causing a large partitioning coefficient once a relatively pure water phase has been created.

Table 6-4. Partitioning of 1-Octene between organic rich phase and the water rich phase of the CO_2 + THF + H_2O system at 298 K. K = C^O (mg/ml) / C^{AQ} (mg/ml)

			Predicted Partition, K	
T (K)	*P* (MPa)	*K* (C^O/C^{AQ})	*HVOS-UNIQUAC*	*HVOS-NRTL*
298	0.2	9	--	--
298	0.3	10	13	--
298	0.5	24	52	--
298	0.7	82	152	6
298	1.0	430	601	52
298	1.4	901	1459	125
298	1.7	2964	2991	250
298	2.6	>3000	9208	820

Modeling of Experimental Results

The Peng-Robinson EoS was chosen to model the phase equilibrium as shown in equation 6-4, where P is pressure, R is the universal gas constant, T is temperature, v is molar volume, and a and b are pure component parameters obtained from equation 6-5 and 6-6, where T_c is the critical temperature and P_c is the critical pressure. The modification of Stryjek and Vera is used to model the temperature dependency of a, equation 6-7, where ω is accentric factor, and κ_1 a pure component parameter fit to the vapor pressure data of the pure component.

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \qquad \text{Eq. 6-4}$$

$$a(T) = 0.457235\frac{RT_c^{\,2}}{P_c}\left(1+\kappa\left[1-\left(\frac{T}{T_c}\right)^{1/2}\right]\right)^2 \qquad \text{Eq. 6-5}$$

$$b = 0.07780\frac{RT_c}{P_c} \qquad \text{Eq. 6-6}$$

$$\kappa = 0.378893 + 1.4897153\omega - 0.17131848\,\omega^2 + 0.0196554\,\omega^3 + \kappa_1\left(1+\frac{T}{T_c}\right)\left(0.7-\frac{T}{T_c}\right) \qquad \text{Eq. 6-7}$$

The pure component parameters for the PRSV EoS are shown in Table 6-5. Several types of mixing rules were tried to fit the binary phase equilibria, including the two parameter van der Waals, the Mathias-Klotz-Prausnitz (Mathias, Klotz et al. 1991) and Huron-Vidal (HV) (Huron and Vidal 1979) type mixing rules. The challenge for these equations is the accurate correlation of the organic + water binary VLE without falsely

predicting the appearance of two liquid phases. Of these mixing rules, only the HV type mixing rules were able to fit the water +organic phase behavior accurately at 298K as shown in Figure 6-7.

The first to successfully use an excess energy based mixing rule with an equation of state was Huron and Vidal (1979). They matched the excess Gibbs free energy from an equation of state with that from an independently prescribed excess Gibbs free energy (g^E) model. They chose a reference pressure of infinity to take advantage of the simplification that at infinite pressure the volume approaches the pure component co-volume parameter b. Their matching procedure yielded the following expression, equation 6-8.

$$\frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} - \frac{1}{\ln 2} \frac{g^{E,\infty}}{RT} \qquad \text{Eq. 6-8}$$

However, the excess Gibbs energy from the EoS is not constant from low pressure to infinite pressure and therefore the available g^E parameters at low pressure cannot be used directly into the expression. To overcome this limitation, recent researchers have reformulated the mixing rules by choosing different reference pressures and/or changing the reference excess energy.

Three modifications of the Huron-Vidal type mixing rules were investigated, modified Huron-Vidal 1 (MHV1) (Michelsen 1990), modified Huron-Vidal 2 (MHV2) (Dahl and Michelsen 1990), and Huron-Vidal-Orbey-Sandler (HVOS) (Orbey and Sandler 1995). The mixing rules are a function of EOS parameters a and b, and excess Gibbs energy (g^E) or excess Helmholtz energy (a^E), found from a liquid activity

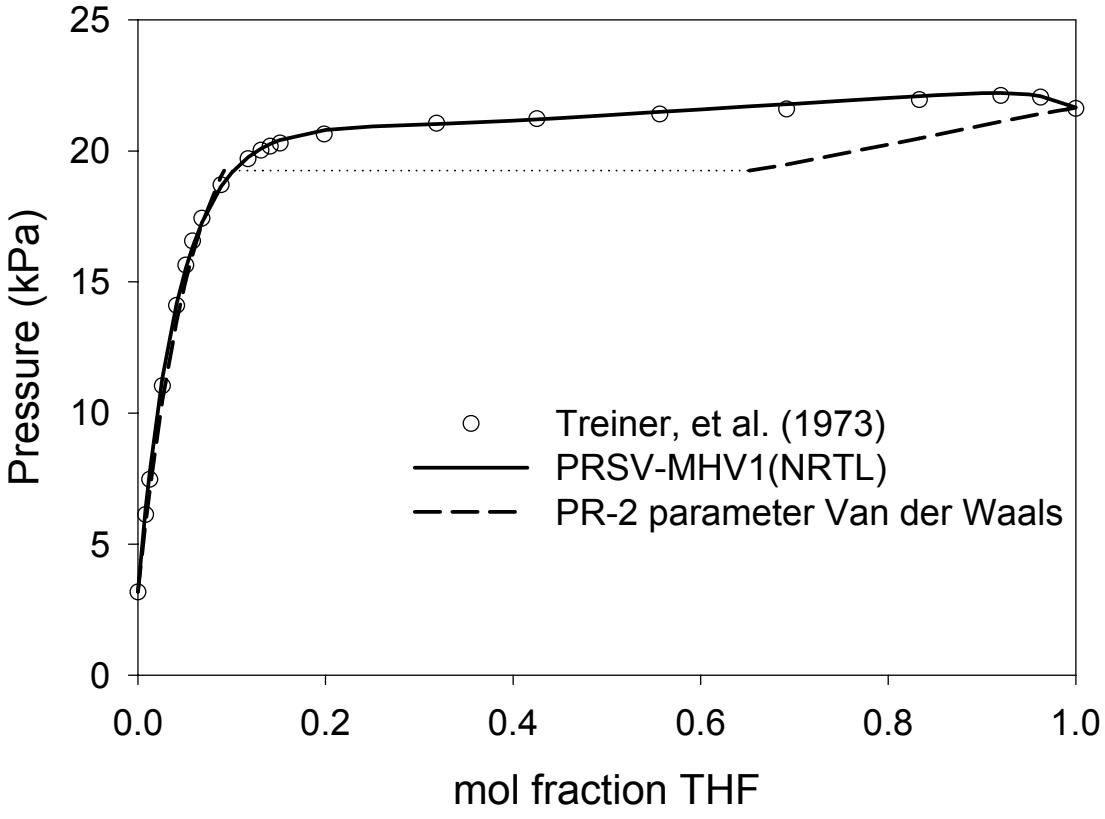

Figure 6-7. P-x diagram of the tetrahydrofuran + water binary system at 298 K with correlations of the PRSV EOS with both MHV1 and a 2-parameter Van der Waals mixing rules.

coefficient model. For convenience the quantity *a/bRT* is replaced by the dimensionless parameter $\alpha = a/bRT$. The MHV1 expression (Eq. 6-9) and the MHV2 expression (Eq. 6-10) are developed by matching the free energy from the EoS to that of an independent liquid activity coefficient model by assuming a reference pressure of zero for both the EoS and the g^E model.

$$\alpha^{MHV1} = \frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} + \frac{1}{q_1^{MHV1}} \left[\frac{g^{E,0}}{RT} + \sum_{i=1}^{n} x_i \ln\left(\frac{b}{b_i}\right) \right] \qquad \text{Eq. 6-9}$$

$$q_1^{MHV2} \left[\alpha^{MHV2} - \sum_{i=1}^{n} x_i \alpha_i \right] + q_2^{MHV2} \left[\left(\alpha^{MHV2}\right)^2 - \sum_{i=1}^{n} x_i \alpha_i^2 \right] = \frac{g^{E,0}}{RT} + \sum_{i=1}^{n} x_i \ln\left(\frac{b}{b_i}\right)$$

Eq. 6-10

The MHV1 model assumes a linear relationship of α for matching energy, whereas the MHV2 model assumes a quadratic relationship to match energy. For the MHV2 model the largest root of α found from the quadratic expression is the mixture α. The *q* parameters are best fit and specific for each EoS; for the PR equation, the values $q_1^{MHV1} = -0.52$, $q_1^{MHV2} = -0.41754$, and $q_2^{MHV2} = -0.0046103$ are used as suggested by Sandler (Orbey and Sandler 1998). Alternately, the HVOS expression (Eq. 6-11), similar to the expression of Wong and Sandler (Wong, Orbey et al. 1992),

$$\alpha^{HVOS} = \frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} + \frac{1}{C^*} \left[\frac{a^{E,\infty}}{RT} + \sum_{i=1}^{n} x_i \ln\left(\frac{b}{b_i}\right) \right] \qquad \text{Eq. 6-11}$$

assumes a reference pressure of infinity. This takes advantage of the pressure independence of excess Helmholtz energy and its relation to the readily obtained g^E, as

shown in equation 6-12. At the limit of infinite pressure the ratio *V/b* goes to unity, therefore $C^* = -0.623225$ for the PR EoS. For all the models used, the

$$g^E(x,T,P=low) = a^E(x,T,P=low) = a^E(x,T,P=\infty) \qquad \text{Eq. 6-12}$$

linear mixing rule was used for the *b* parameter, as shown in equation 6-13.

$$b = \sum_i x_i b_i \qquad \text{Eq. 6-13}$$

One excess free energy model that was used in the mixing rule expressions is the NRTL (Renon and Prausnitz 1968) model, shown in equation 6-14 and 6-15,

$$\frac{g^E}{RT} = \sum_i^n x_i \frac{\sum_{j=1}^n \tau_{ji} G_{ji} x_j}{\sum_{k=1}^n G_{ki} x_k} \qquad \text{Eq. 6-14}$$

where

$$\tau_{ji} = \frac{\Delta g_{ji}}{RT} \qquad \text{and} \qquad G_{ji} = \exp\left(-\alpha_{ji}\tau_{ji}\right), \qquad \text{Eq. 6-15}$$

and where the Δg_{ji} is the energy parameter and the α_{ji} term is the non-randomness parameter. Also the UNIQUAC (Abrams and Prausnitz 1975) model was used, as shown in equations 6-16 and 6-17,

$$\frac{g^E}{RT} = \sum_{i=1}^n x_i \ln\frac{\Phi_i}{x_i} + \frac{z}{2}\sum_{i=1}^n q_i x_i \ln\frac{\theta_i}{\Phi_i} - \sum_{i=1}^n q_i x_i \ln\sum_{j=1}^n \theta_j \tau_{ji} \qquad \text{Eq. 6-16}$$

$$\Phi_i = \frac{r_i x_i}{\sum_{j=1}^n r_j x_j} \qquad \theta_i = \frac{q_i x_i}{\sum_{j=1}^n q_j x_j} \qquad \tau_{ij} = \exp\left(-\frac{u_{ij}}{RT}\right) \qquad \text{Eq. 6-17}$$

where u_{ij} is the interaction energy parameter; r and q are the pure component volume and area terms, respectively; and z is the coordination number set equal to 10.

In this work a comparison of the two mixing rules with both the NRTL and UNIQUAC g^E models were used to correlate the seven binary systems that constitute the solvent systems. The energy parameters for the g^E model were fit to the VLE data of the binary systems by minimizing the sum of squares error in pressure; the results are shown in Table 6-6. In the case of the NRTL model, the α_{ij} was set to 0.2, except for the organic + water systems where α was regressed along with the other two parameters. The binary systems fit with available temperature range were as follows: carbon dioxide + tetrahydrofuran from 298 to 333 K (Lazzaroni, Bush et al. 2004), tetrahydrofuran + water from 298 to 343 K (Signer, Arm et al. 1969; Matous, Novak et al. 1972; Treiner, Bocquet et al. 1973) , carbon dioxide + water from 298 to 353 K (Wiebe and Gaddy 1940; Bamberger, Sieder et al. 2000), carbon dioxide + acetonitrile at 313 K (Kordikowski, Schenk et al. 1995), acetonitrile + water from 303 to 323 K (Vierk 1950; Wilson, Patel et al. 1979; Villamanan, Allawi et al. 1984) , carbon dioxide + 1,4-dioxane at 313 K (Kordikowski, Schenk et al. 1995), and 1,4-dioxane + water from 308 to 323 K (Hovorka, Scheafer et al. 1936; Steinbrecher and Bittrich 1963; Kortuem and Valent 1977; Balcazar-Ortiz, Patel et al. 1979; Loehe, Van Ness et al. 1981). The average absolute deviation (AAD) in pressure is reported for each of the correlated binaries in Table 6-7; the MHV1-NRTL and HVOS-NRTL were best able to fit the binary VLE of the systems in this study. When VLE was not available at the temperature of interest, the binary parameters were interpolated from the available data.

Table 6-5. Pure component parameters used in the PRSV EOS.

Compounds	T_c (K)	P_c (bar)	ω	κ_1	r	q
CO_2	304.21	73.6	0.2250	0.04285	1.299	1.292
H_2O	647.13	220.55	0.3438	-0.06635	0.920	1.400
Tetrahydrofuran	540.15	51.9	0.2255	0.03961	2.866	2.172
Acetonitrile	545.5	48.3	0.3371	-0.13991	1.870	1.724
1,4-Dioxane	587	52.08	0.2793	0.02013	3.073	2.360
1-Octene	567	26.8	0.3921	0.00165	5.618	4.724

Table 6-7. Deviation in pressure ($\Delta P/P$ x 100%) for the mixing rule models.

		HVOS		MHV1		MHV2	
System	T Range (K)	UNIQ	NRTL	UNIQ	NRTL	UNIQ	NRTL
CO_2 + THF	298-333	2.27	2.27	1.20	1.51	0.63	0.74
THF + H_2O	298-343	1.60	0.86	1.52	0.70	1.95	0.65
CO_2 + H_2O	298-353	4.35	2.84	3.61	2.82	2.94	2.56
CO_2 + ACN	313	3.60	3.48	4.19	3.41	4.36	3.41
ACN + H_2O	306-323	1.50	0.40	1.42	0.31	1.57	0.67
CO_2 + DIOX	313	14.87	16.35	9.27	13.42	6.80	11.05
DIOX + H_2O	308-323	2.09	0.62	2.43	0.56	3.35	0.57

Table 6-6. Optimized mixing parameters used in the MHV1, MHV2, & HVOS mixing rule with both NRTL and UNIQUAC g^E models.

		MHV2			MHV1			HVOS		
		NRTL		UNIQUAC	NRTL		UNIQUAC	NRTL		UNIQUAC
System	T (K)	$\Delta g_{12}/\Delta g_{21}$ (cal/mol)	α	U_{12}/U_{21} (cal/mol)	$\Delta g_{12}/\Delta g_{21}$ (cal/mol)	α	$\Delta U_{12}/\Delta U_{21}$ (cal/mol)	$\Delta g_{12}/\Delta g_{21}$ (cal/mol)	α	U_{12}/U_{21} (cal/mol)
CO_2 + THF	298	333/-351	0.2	200/-200	1306/-1071	0.2	-346/294	301/-493	0.2	-138/2.5
	313	267/-279	0.2	172/-172	1117/-956	0.2	-223/149	596/-652	0.2	99.5/-180
	333	521/-562	0.2	309/-309	637/-714	0.2	-81.8/-39.1	748/-832	0.2	458/-458
THF + H_2O	298	1122/1505	0.416	1043/-242	970/1110	0.528	1528/-470	1199/1442	0.406	1230/-271
	313	1063/1656	0.416	915/-213	1012/1303	0.528	1374/-443	1272/1686	0.406	1073/-204
	333	990/1851	0.416	774/-159	1070/1558	0.528	1193/-407	1372/2009	0.406	896/-120
CO_2 + H_2O	298	3525/1437	0.2	8118/1133	1916/565	0.2	791/605	2620/1065	0.2	856/978
	313	3651/1421	0.2	8118/1113	2561/622	0.2	821/651	3022/1102	0.2	1448/953
	333	3843/1425	0.2	8118/1109	3408/692	0.2	862/712	3148/1103	0.2	1775/898
CO_2 + ACN	313	894/-522	0.2	233/-49.8	1707/-1094	0.2	845/-467	1894/-1124	0.2	968/-472
ACN + H_2O	313	814/1448	0.418	306/447	821/1120	0.546	311/221	990/1489	0.409	383/454
CO_2 + DIOX	313	705/-785	0.2	387/-387	898/-1033	0.2	493/-493	979/-1136	0.2	567/-567
DIOX + H_2O	313	537/876	0.287	1583/-507	737/456	0.353	1668/-581	649/883	0.267	1957/-490
CO_2 + 1-Octene	298	378/-27.6	0.2	190/137	1883/-1140	0.2	238/53.3	2240/-1146	0.2	352/43.5
THF + 1-Octene	298	762/-417	0.2	-124/251	762/-417	0.2	-124/251	762/-417	0.2	-124/251
H_2O + 1-Octene	298	7718/3875	0.2	1042/2666	7718/3875	0.2	1042/2666	7718/3875	0.2	1042/2666

To predict the partition coefficient of 1-octene, the energy parameters for the water + 1-octene binary system were fit to mutual solubility data (Economou, Heidman et al. 1997). For the carbon dioxide + 1-octene system, the carbon dioxide + octane VLE data (Weng and Lee 1992) were used in lieu of available data. It is not expected for there to be a substantial difference between the VLE of the two systems, therefore the 1-octene pure component parameters were used with the VLE data for octane system for the regression of parameters. For the tetrahydrofuran + 1-octene binary, energy parameters for the excess energy model were fit to the predicted infinite dilution activity coefficients predicted using both the MOSCED (Thomas and Eckert 1984) model and the Modified UNIFAC-Dortmund (Gmehling, Li et al. 1993) model. Both models gave essentially the same activity coefficients of $\gamma_{THF}^{\infty} = 1.3$ and $\gamma_{1-Octene}^{\infty} = 1.6$, where the subscript denotes the dilute species.

The model predictions and experimental data for the carbon dioxide + tetrahydrofuran + water LLE at 298 K, 313 K, and 333 K are shown in Figures 6-8, 6-9 and 6-10. The best predictions were achieved by the HVOS and MHV1 mixing rules with the UNIQUAC g^E model, with the best prediction at 298 K being with the HVOS-UNIQUAC model. For all the different mixing rules used with the NRTL equation, the models over-predicted the purity of the organic-rich phase. The good agreement of the predicted isobaric tie-lines with the experimental tie-lines demonstrates the ability of the models to capture the pressure dependence. As the temperature is increased from 298 K to 333 K the pressure required for a comparable phase split was increased also. Above 298 K all the models incorrectly predict a phase split for the tetrahydrofuran + water

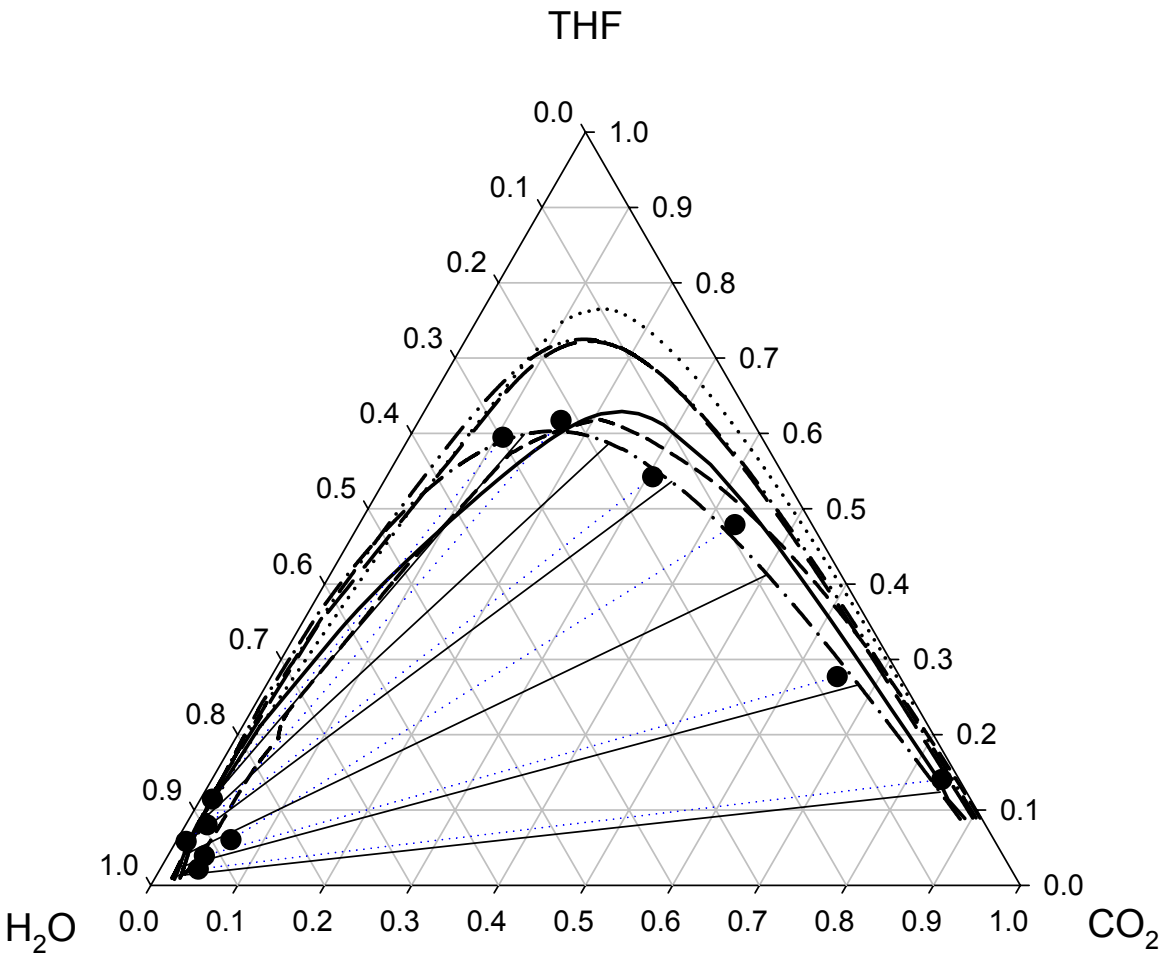

Figure 6-8. Prediction of the LLE of CO_2 + Tetrahydrofuran (THF) + H_2O at 298 K. (●) Experimental data, this work. MHV1 (UNI———— , NRTL— — —) ; MHV2 (UNI– – – –, NRTL.....); HVOS (UNI— . —, NRTL— . . —). Isobaric tie-lines, experimental are dotted, and solid are predicted using HVOS-UNIQUAC.

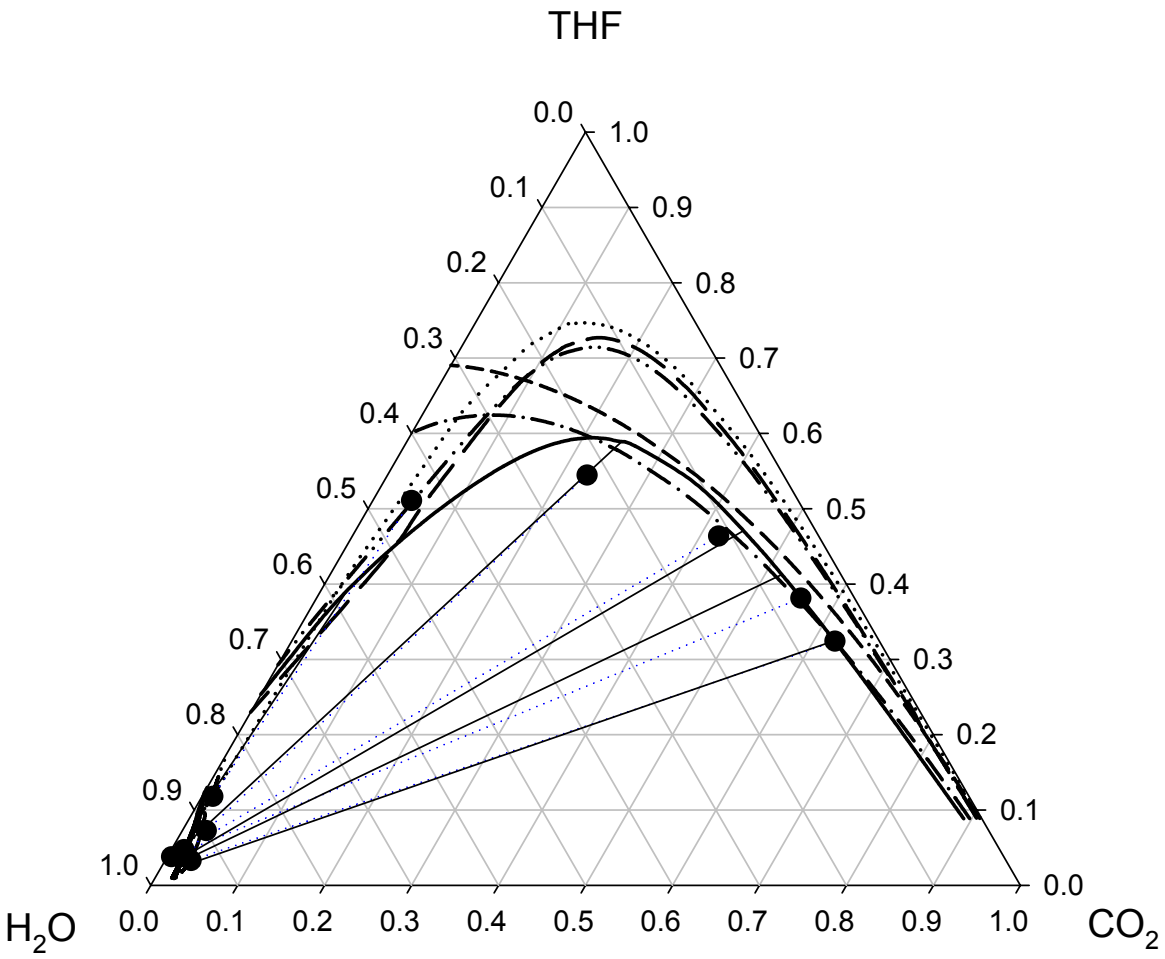

Figure 6-9. Prediction of the LLE of CO_2 + Tetrahydrofuran (THF) + H_2O at 313 K. (●) Experimental data, this work. MHV1 (UNI———— , NRTL— — — .) ; MHV2 (UNI— — — —, NRTL.....); HVOS (UNI— . —, NRTL— . . —). Isobaric tie-lines, experimental are dotted, and solid are predicted using MHV1-UNIQUAC.

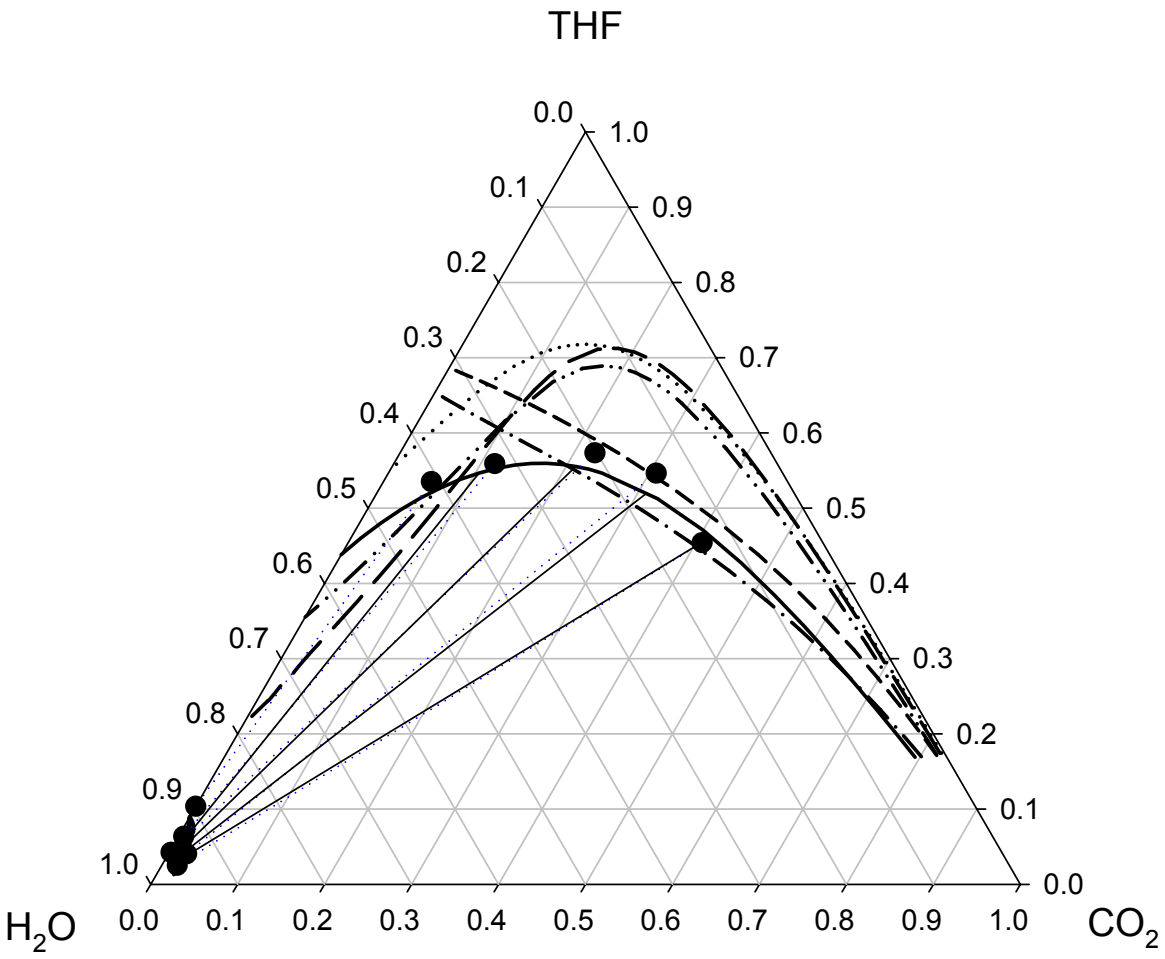

Figure 6-10. Prediction of the LLE of CO_2 + Tetrahydrofuran (THF) + H_2O at 333 K. (●) Experimental data, this work. MHV1 (UNI———— , NRTL— — — .) ; MHV2 (UNI– – – –, NRTL.....); HVOS (UNI— . —, NRTL— . . –). Isobaric tie-lines, experimental are dotted, and solid are predicted using MHV1-UNIQUAC.

binary, however the models are still able to fit the LLE at carbon dioxide concentrations greater than 10% in the organic rich phase.

For the carbon dioxide + acetonitrile + water LLE at 313 K, the mixing rules using the NRTL g^E model predict the experimental data the best, with the HVOS-NRTL fitting slightly better than the other models, as show in Figure 6-11. The mixing rules using the UNIQUAC model falsely predict a phase split for the acetonitrile + water binary and do not capture the type I behavior expected. For the CO_2 + 1,4-dioxane + water LLE at 313 K, none of the mixing rules give the correct prediction, with the mixing rules using the NRTL equations giving the most reasonable results, as shown in Figure 6-12. The poor fit of the 1,4-dioxane + water binary by the models using the UNIQUAC equation, and the poor fit of the carbon dioxide + 1,4-dioxane binary by the models using the NRTL equation contributed most to the inaccuracy of the prediction.

The HVOS-UNIQUAC model is best able to predict the partitioning of 1-octene between the organic and aqueous phases, as shown in Table 6-4. This is not surprising since this model was best able to predict the compositions and pressures of the LLE in the ternary CO2 + THF + water system. The HVOS-NRTL model does not predict a phase split at pressures lower than 0.5 MPa, and therefore cannot predict a partition coefficient. Since the 1-octene is present in finite concentrations, at the low pressure point of 0.2 MPa the amount of 1-octene present in the experiment may have lowered the immiscibility pressure causing a phase split were none would have occurred in the ternary system.

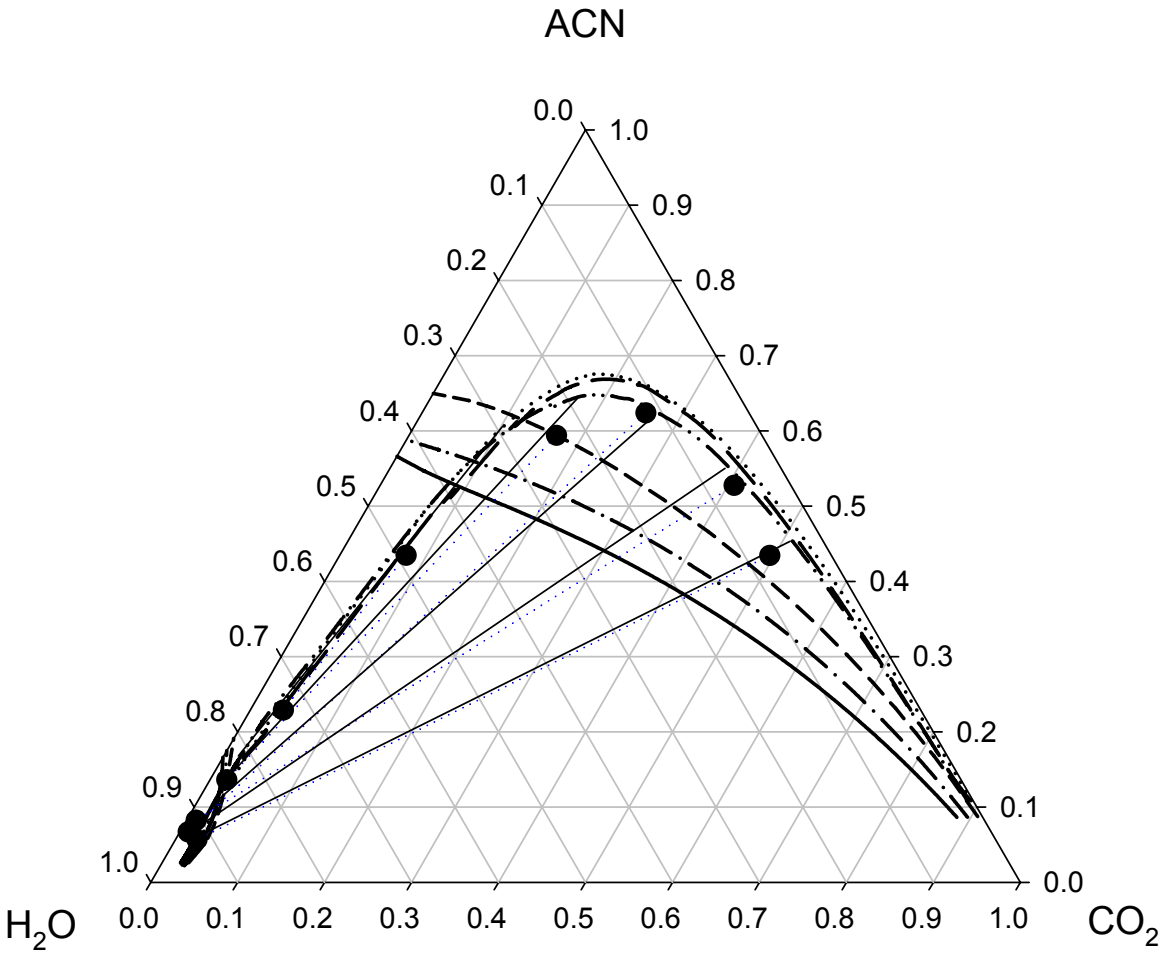

Figure 6-11. Prediction of the LLE of CO_2 + Acetonitrile (ACN) + H_2O at 313 K. (●) Experimental data, this work. MHV1 (UNI———— , NRTL— — —) ; MHV2 (UNI— — — —, NRTL.....); HVOS (UNI— . —, NRTL— . . —). Isobaric tie-lines, experimental are dotted, and solid are predicted using HVOS-NRTL.

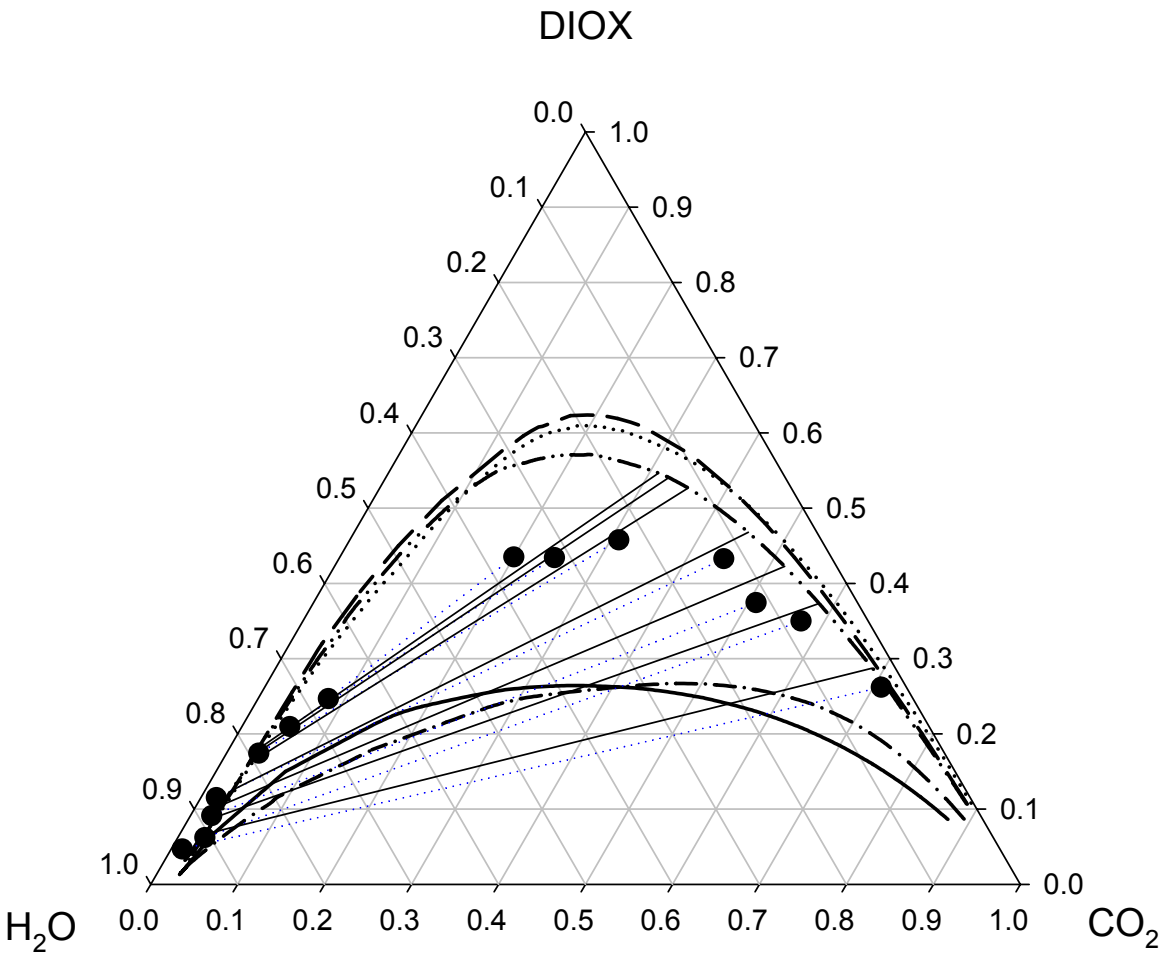

Figure 6-12. Prediction of the LLE of CO_2 + 1,4-Dioxane (DIOX) + H_2O at 313 K. (●) Experimental data, this work. MHV1 (UNI———— , NRTL— — .) ; MHV2 (NRTL.....); HVOS (UNI— . —, NRTL— . . —). Isobaric tie-lines, experimental are dotted, and solid are predicted using HVOS-NRTL.

Summary

We have shown a potential solvent system that is a modification to the traditional aqueous biphasic system for sequestration and recycle of homogeneous catalysts. The addition of a polar organic solvent that is miscible with the aqueous phase allows for the reaction to be carried out in a single phase. We have shown that upon addition of modest pressures of carbon dioxide to the system a phase split occurs forming both water-rich and organic-rich phases. The LLE for three polar organic solvents, tetrahydrofuran, acetonitrile, or 1,4-dioxane with water and carbon dioxide are reported. The tetrahydrofuran + water system requires the smallest amount of carbon dioxide (lower pressures) to cause a phase split sufficient for catalyst sequestration. The phase split of the acetonitrile + water system with carbon dioxide results in a less pure aqueous phase, although it still may be sufficient for catalyst separation with the addition of more carbon dioxide. The greater affinity of 1,4-dioxane to water increases the amount added carbon dioxide necessary for a phase split and results in less pure phases than the other systems. The partitioning of the reactant for a hydroformylation reaction (1-octene) is sufficient for separation of the reactant from the tetrahydrofuran + water mixture.

The PRSV EoS with modified Huron-Vidal mixing rules have been shown to predict well the ternary and quaternary phase behavior of these systems from only the correlated binary VLE and LLE. The key binary systems for the solvent mixtures studied here are the polar organic solvent + water system. For the chosen model to perform well it must accurately represent the VLE of this strongly non-ideal system over the required temperature range. The models are able to predict the partitioning of the reactant 1-

octene between the equilibrium phases well, when the VLLE behavior of the solvent system is predicted well.

Nomenclature

a = equation of state attractive parameter
a^E = excess Helmholtz energy
b = equation of state volume parameter
C^* = mixing rule constant
g^E = excess Gibbs energy
Δg_{ji} = NRTL energy parameter (cal/mol)
G_{ji} = NRTL parameter
n = number of components
P = pressure
q_1, q_2 = mixing rule constants
q = UNIQUAC pure component area parameter
r = UNIQUAC pure component volume parameter
R = universal gas constant
T = temperature
u_{ij} = UNIQUAC energy parameter (cal/mol)
x = mole fraction composition
z = coordination number (set to 10)

Greek

α = equation of state parameter, a/bRT
α^{NRTL} = NRTL nonrandom parameter
Φ = UNIQUAC segment fraction
θ = UNIQUAC area fraction
τ = parameter used in eq. 6, 7 and eq. 8, 9

Superscripts

0 = zero pressure reference state
∞ = infinite pressure reference state

Subscripts

i,j = component indices

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CHAPTER VII

SOLUBILITY OF SOLIDS IN GAS-EXPANDED LIQUIDS

Introduction

There is much recent interest in the use of supercritical fluid processes to control the particle design of pharmaceutical, cosmetic, specialty chemicals, and other fine materials, including explosives, polymers, and catalysts. In the case of pharmaceutical compounds, control of particle morphology, particle size, and size distribution are important factors in improving the efficiency and efficacy of pharmaceutical compounds. Micronization of products can often lead to more direct delivery of the drug, lower doses with the increased efficiency, and better bioavailablity with controlled release (Shariati and Peters 2003). Current techniques for making products on the micron scale, include jet and ball milling, spray drying, and liquid evaporation or liquid anti-solvent, and often do not give the required particle size control, and may require high operating temperatures that can lead to thermal degradation of the product, as is the case with some spray drying processes (Shariati and Peters 2002). Use of supercritical fluid processes have been shown useful at producing smaller and better defined particles with smaller size distributions than current methods.

There have been several reviews that cover the recent developments and applications of high pressure solvent systems to particle formation and solids processing

(Jung and Perrut 2001; Dehghani and Foster 2003; Shariati and Peters 2003). The two main techniques used for micronizing materials are rapid expansion of supercritical solutions (RESS) process and gas (or supercritical fluid) anti-solvent recrystallization (GAS or SAS).

In the RESS process, a supercritical fluid is saturated with the substrate(s) of interest at a high pressure, and then through a heated nozzle the solution is expanded into a low pressure vessel, causing a rapid decrease in the solubility of the substrate in the solvent and rapid nucleation to form very small particles. Fine particles (0.5-20 μm) with very narrow size distributions have been demonstrated. This method of micronization is very attractive because it eliminates the need for an organic solvent. One of the major drawbacks of this process however, is the low solubility of substrates in the supercritical phase. The solubility of the substrate can be increased in the supercritical phase by the addition of organic co-solvents, although the organic may be incorporated into the final powder. Using RESS several different polymer fibers including, PMMA (Matson, Fulton et al. 1987) and polystyrene (Petersen, Matson et al. 1987) have been produced, as well as a some inorganic compounds, including metal films (Hansen, Hybertson et al. 1992) and a variety of organics including pharmaceutical compounds (Debenedetti, Tom et al. 1993; Reverchon, Donsi et al. 1993; Frank and Ye 2000).

More recent effort has been focused on the use of mixed solvent system to produce fine particles. In contrast to the RESS process, the GAS/SAS process uses a supercritical fluid or high pressure gas as an anti-solvent to precipitate the substrate out of solution. As shown in Figure 7-1, in this batch process an organic solvent is saturated

with the substrate is added to a precipitation vessel, and the anti-solvent is added, to the top of the liquid or bubbled through to enhance mass transfer. The addition of the anti-solvent causes a decrease in the solvating power of the solution, causing precipitation of the substrate, which is then collected on the filter.

A variation of the GAS process is aerosol solvent extraction system (ASES), shown in Figure 7-2. In this process a solution of substrate and organic solvent are atomized through a nozzle into a vessel filled with compressed anti-solvent. Typically the solution is introduced into the vessel at a pressure around 20 bar greater than the operating pressure. The rapid dissolution of the anti-solvent into the atomized droplets causes a decrease in the solvent power of the liquid, resulting in supersaturation of the liquid and precipitation of small and usually uniform particles. The formed particles are collected on a filter and the mixture of solvent and anti-solvent are separated by depressurization in a low pressure vessel.

One of the first applications of the GAS process was the recrystallization of explosive compounds by Gallagher et al. (Gallagher, Coffey et al. 1989) who demonstrated control over crystal morphology and size distribution with control of anti-solvent addition. More recently the GAS/SAS and ASES process has been applied to many other compounds, including: biopolymers, like HYAFF 7 have been recrystallized from DMSO with CO_2 (Pallado, Benedetti et al. 1996); very small polymer particles of 1 μm were achieved for micronization of PLGA from acetone (Dillow, Dehghani et al. 1997); inorganic salts have been recently been crystallized from DMSO solution with CO_2 (Yeo, Choi et al. 2000), as well as metallocene compounds like yttrium acetate

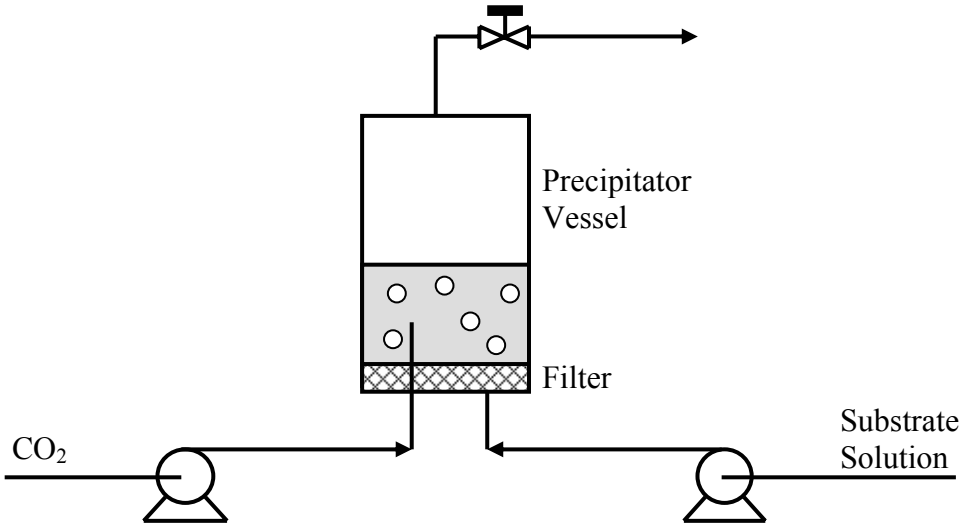


Figure 7-1. GAS/SAS process concept diagram.

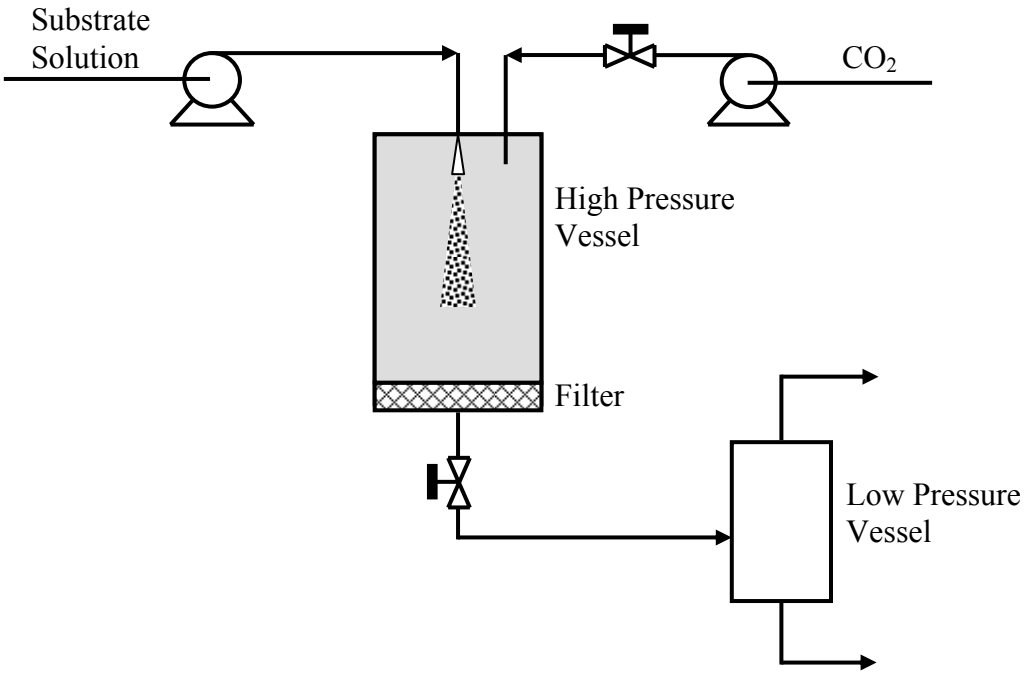


Figure 7-2. ASES process concept diagram.

(Reverchon, Porta et al. 1997) (Muhrer, Dörfler et al. 2000); many different pharmaceutical compounds, including acetaminophen (Gilbert, Palakodaty et al. 2000), amoxicillin (Reverchon, Porta et al. 1999), and Naproxen (Chou, 1997) have been micronized; Theiring, et al. (Thiering, Dehghani et al. 2000) recently crystallized several proteins from a variety of organic solvents using CO_2; and microcomposites of polymer with active substrates have been achieved (Pallado, Benedetti et al. 1996) (Elvassore, Bertucco et al. 2000).

Other variations of anti-solvent processes have been developed using nozzles for atomization and particle production. Researchers at Bradford University developed a method known as solution enhanced dispersion by supercritical fluids (SEDS) (Hanna and York 1994), where the anti-solvent and solution of substrate are introduced into a precipitation vessel through coaxial nozzles. Here the supercritical fluid anti-solvent has both a chemical and mechanical "spray enhancer" effect on the particle formation; the supercritical fluid breaks up the liquid solution into small droplets that precipitate. A variation of this has been developed by researchers at the University of Kansas (Subramaniam, Said et al. 1997) that uses a novel nozzle design to produce sonic waves that breaks up the liquid into small particles of around 1 μm. Another variation of the anti-solvent process is the depressurization of expanded liquid organic solvent (DELOS) process (Ventosa, Sala et al. 2003). In the DELOS process, the substrate is dissolved in a high pressure mixture of organic solvent and compressible fluid and then rapidly depressurized to atmospheric pressure, causing a large drop in temperature upon expansion of the fluid and resulting in the formation of particles.

An interesting combination of reaction with anti-solvent precipitation proposed by Owens, et al. (Owens, Anseth et al. 2002) (Owens, Anseth et al. 2003) is the compressed anti-solvent precipitation and photopolymerization (CAPP) process. In this process, similarly to the ASES process, monomer and photoinitiator are dissolved in an organic solvent and sprayed into a compressed gas anti-solvent while the vessel is illuminated with high-intensity ultraviolet light. The good mixing of all components is achieved by the spraying action; while the anti-solvent may be extracting the organic from the liquid droplet increasing the concentration of the photoinitiator and monomer and also precipitating the polymer particles as they are forming.

Carbon dioxide is most often chosen as the anti-solvent or solvent (in the case of RESS) because it offers many advantages to other organic fluids: it is non-toxic, (especially important for pharmaceutical products), non-flammable, and inexpensive. The low critical properties (T_c = 304.2 K, P_c = 73.8 bar) make the supercritical state easily accessible, and the miscibility in many organic solvents making it applicable to many solvent system. The low viscosity and good mass transport properties make it very useful for the crystallization processes.

For the GAS process, most of the current research has focused on the process variables including the effects of temperature, pressure, rate of anti-solvent addition, product morphology, and size and size distribution. As Peters (Shariati and Peters 2002) and Reverchon (Reverchon, Caputo et al.) point out, the role of phase behavior of the ternary solution is also important for the control of morphology and for process characterization. Knowledge of the phase behavior can be drastically affected by choice

of solvent and anti-solvent and can be key factors in the optimization of the overall process. There is a limited amount of data available in the literature of ternary phase behavior for organic solids with mixtures of a solvent and an anti-solvent across a large pressure or composition range. The available data include: the solubility of salicylic acid in 1-propanol + carbon dioxide (Shariati and Peters 2002); the solubility of a colorant in acetone + carbon dioxide (Ventosa, Sala et al. 2003); the solubility of acetaminophen in 1-butanol + carbon dioxide and the solubility of β-carotene in toluene + carbon dioxide (Chang and Randolph 1990); the solubility of hydroxybenzoic acid isomers in ethyl acetate + carbon dioxide (Liu, Li et al. 2000); the solubility of cholesterol in acetone + carbon dioxide (Liu, Wang et al. 2002); the solubility of o- and p-aminobenzoic acids in ethanol + carbon dioxide (Liu, Yang et al. 2000); and the solubility of phenanthrene and naphthalene in toluene + carbon dioxide (Dixon and Johnston 1991). Given the available data, there has been little effort to measure the solubility of a single solute in several organic solvents to examine the effect of the solvent choice upon the ternary phase behavior.

To compare the effect of liquid solvent upon the phase behavior of a solid organic in carbon dioxide expanded liquids, the solubilities of phenanthrene and acetaminophen, chosen as model pharmaceutical compounds, in several organic solvents are investigated. The solubility of phenanthrene in toluene, acetone, or tetrahydrofuran with carbon dioxide mixtures were investigated at 298 K up to a pressure of 5.8 MPa. The solubility of acetaminophen in ethanol or acetone with carbon dioxide mixtures were investigated at 298 K up to a pressure of 5.8 MPa. .

The role of the anti-solvent on the phase behavior is also considered. The anti-solvent power of hexane is compared to that of carbon dioxide for acetaminophen + ethanol system. Some insights into the interactions in the liquid phase are gained through comparison of the phase equilibria.

The ternary phase behavior is predicted using the binary infinite dilution activity coefficients predicted using the MOSCED model. In addition to the ternary system, the MOSCED model is used to predict the carbon dioxide + organic binary VLE, and the solubility of solids in supercritical carbon dioxide. Given the predicted activity coefficients, two approaches to calculating the phase behavior are used: the Peng-Robinson equation of state with Stryjek-Vera modification with g^E based mixing rules ; and γ–ϕ approach, where a liquid activity coefficient model is used to describe the liquid phase and an equation of state is used for the vapor phase.

Experimental Materials

Solid components phenanthrene (98%) and acetaminophen (98%) were obtained from Aldrich Chemical Company and were used as received. Liquid components acetone (HPLC 99%), tetrahydrofuran (HPLC 99%), toluene (HPLC 99%), hexane (anhydrous), ethanol (anhydrous), and ethyl acetate (ACS 99.8%) were obtained from Aldrich Chemical Co. and were used as received. SFC Grade carbon dioxide (99.99%) was obtained from Matheson Gas Products. The CO_2 was further purified to remove trace water using a Matheson (Model 450B) gas purifier and filter cartridge (Type 451).

Apparatus and Procedure

Experimental Apparatus

A schematic of the equilibrium cell apparatus is shown in Figure 7-3. The equilibrium cell is a transmission type sight gauge (Jerguson Model 18T-32). The equilibrium cell was placed in a temperature controlled air bath. The temperature of the air bath and vapor phase inside the cell was monitored with a thermocouple (Omega Type K) and digital readout (HH-22 Omega). The air bath temperature was maintained by a digital temperature controller (Omega CN76000) with an over temperature controller (Omega CN375) for safe operation. The temperature was accurate to within ±0.2 K and calibrated against a platinum RTD (Omega PRP-4) with a DP251 Precision RTD Benchtop Thermometer (DP251 Omega) accurate to ±0.025 K and traceable to NIST. The pressures were measured with a pressure transducer and digital read-out (Druck, DPI 260, PDCR 910). The transducer was calibrated against a hydraulic piston pressure

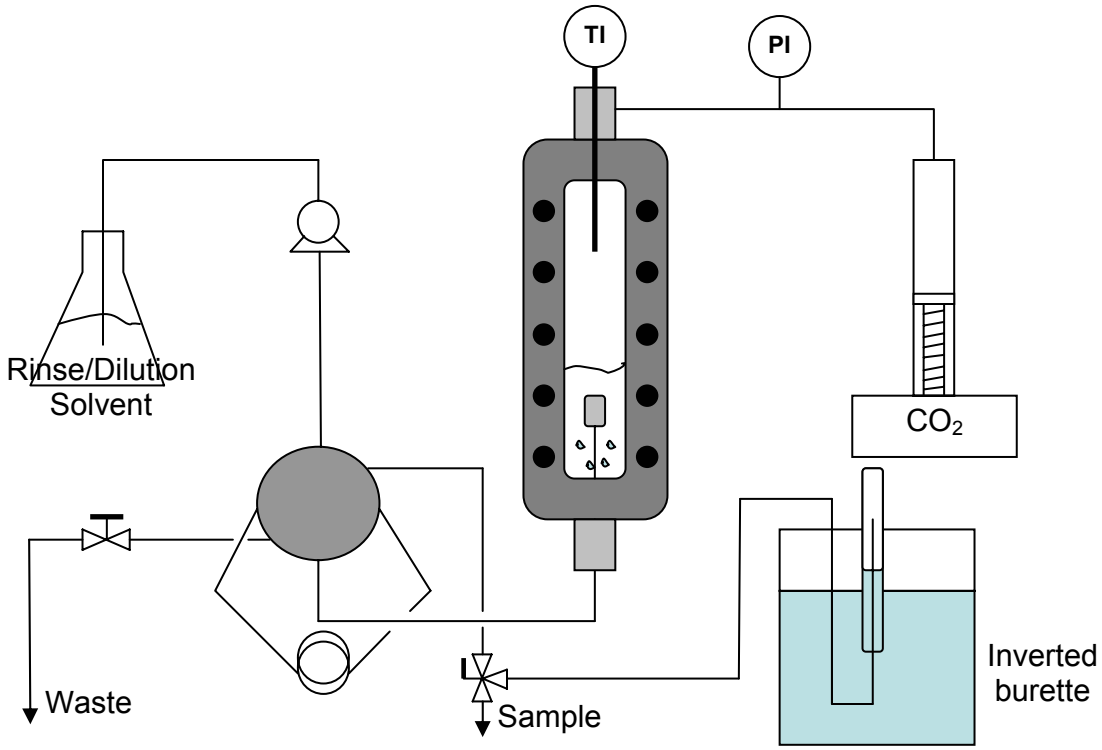


Figure 7-3. Schematic of experimental apparatus.

gauge (Ruska) to an uncertainty of +/- 0.1 bar. The cell is mounted on a rotating shaft, and mixing is achieved by rotating the entire cell.

CO_2 was metered into the cell from a high pressure syringe pump (Isco Model 260D). Because there is a free-floating solid phase in the vessel a sintered metal frit was attached to the sampling line to prevent capture of solid particles into the sample loop. To remove a representative sample from the equilibrium liquid phase of the cell contents a six-way sampling valve (Valco) was used. This is a two position valve and its operation is discussed in the procedure section below. The sample loop with a volume of 50 uL was found to be sufficiently small to prevent any pressure drop in the cell and large enough for facile analysis. The rinse/dilution solvent was pumped by a high pressure liquid pump. In this study ethyl acetate was used as the rinse/dilution solvent.

Experimental Procedure

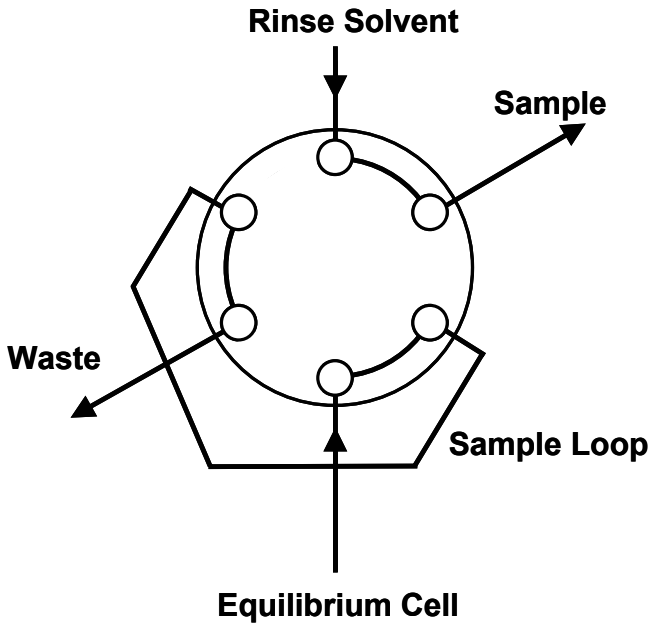
The cell is initially loaded with a liquid organic solvent saturated with the solid solute. Some additional solid solute is added to assist the crystallization process and prevent the system from being super-saturated. Carbon dioxide is then added to the cell and the cell is thoroughly mixed. The cell contents are allowed to rest for approximately 30 minutes before a sample is taken.

The 6-way sample valve can be in two positions as shown in Figure 7-4. The valve starts in position B and the rinse solvent is pumped to completely fill the sample loop. This is done to prevent any change in pressure that could cause flashing of the carbon dioxide or solid phase falling out of solution. The sample valve is then moved to

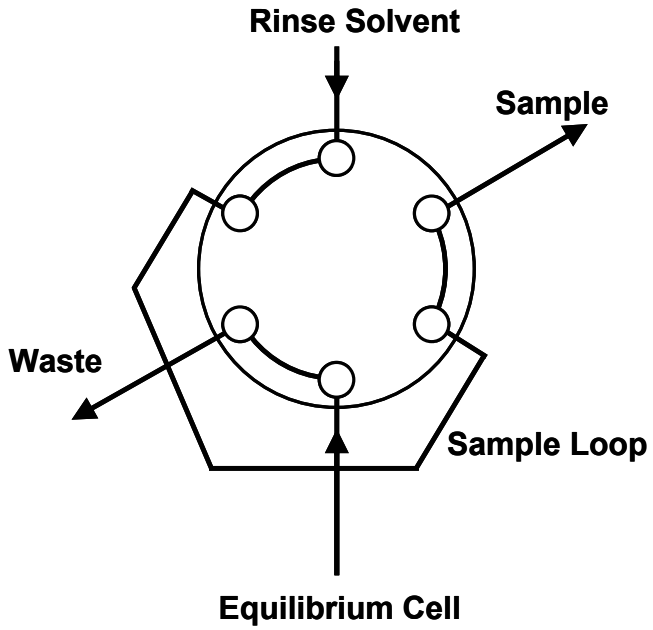
position A, where the cell contents can now flow into the sample loop. The two-way valve on the waste line (initially closed) is opened to remove the solvent and allow the cell contents to flow into the sample loop. A small diameter tube is used to restrict the flow of the cell contents with the end of the tube placed in liquid water. The cell contents are allowed to flow through the sample loop until a steady stream of bubbles are seen in the water. While this does disturb the cell slightly, only a small change in pressure is seen (approximately 1 psia for 3 samples).

The sample valve is now moved back to position B; the sample is depressurized into a vial of known mass and bubbled through a portion of the dilution solvent. The sample is diluted with approximately 10 ml of ethyl acetate and is weighed to determine the amount of dilution solvent added (neglecting sample contribution). The sampling is repeated three times for each pressure. The samples are analyzed by GC-FID to determine the concentration of the solid solute and the organic solvent. Additional samples are required to determine the amount of carbon dioxide in the sample.

The capture of the sample in the sample loop is the same for the determination of carbon dioxide concentration. The 3-way valve on the sample line, instead of being depressurized into the dilution solvent, is diverted to an inverted burette placed in a water bath. The volume of carbon dioxide at STP is determined by the displacement of water in the burette. The sample should not be bubbled through the water as there is an appreciable solubility of carbon dioxide in the water. Without any mixing the rate of dissolution of carbon dioxide into the water is slow enough to be negligible so long as the volume is rapidly determined. The line is flushed with rinse solvent to ensure all the



POSITION A



POSITION B

Figure 7-4. The 2 possible positions of the sample valve. Position A for loading the sample loop and Position B for collecting the sample for analysis.

carbon dioxide is in the burette. The sampling is repeated three times and the results averaged to mitigate error in the sampling procedure.

To test the accuracy of the method, the solubility of phenanthrene in a mixture of toluene and carbon dioxide was examined and compared to the literature data of Johnston, et al. (Dixon and Johnston 1991). The results compare very well with the literature data and are shown in Figure 7-5.

The solubility data at the highest pressures or lowest phenanthrene concentrations were not possible with this experimental set-up. The practical limit of this method and apparatus is to about 0.001 mol fraction of the solid solute. It would be possible to quantify the lower concentrations with a larger sample loop or less dilution rinse. Although with less dilution solvent the risk of not capturing all the solute becomes greater. The range of this method is still large enough to capture any unique phase behavior that is occurring in other solvent systems. This method is limited to systems where the solute has much higher solubility in the organic solvent than it does in the carbon dioxide.

The solubility of solids in ambient pressure mixtures of organic solvents followed the experimental procedure from Chapter III. In short, the equilibrium vial is placed in a temperature controlled water bath and allowed to equilibrate for 24 hours. A sample of liquid phase is removed and diluted to allow for GC analysis.

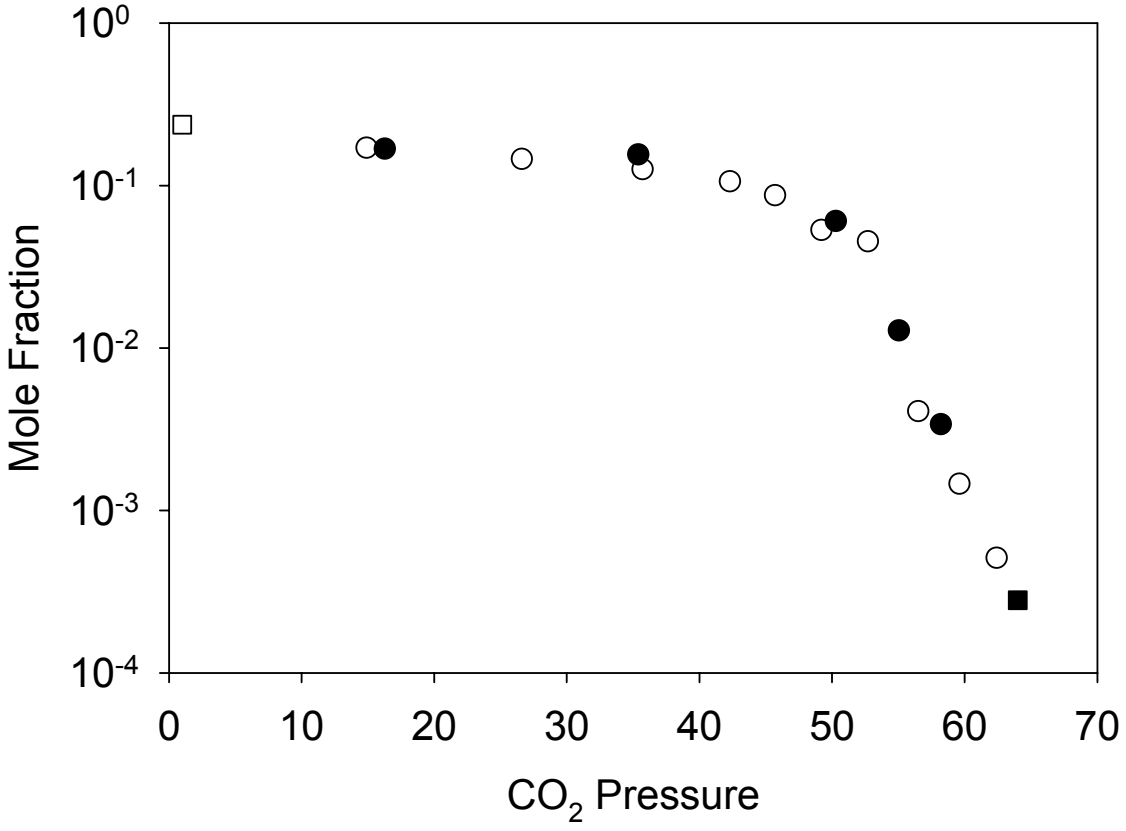


Figure 7-5. Solubility of phenanthrene in carbon dioxide + toluene mixture versus carbon dioxide pressure. Literature data (○),(■) (Dixon and Johnston 1991), (□)(Acree and Abraham 2001), and this work (●).

Experimental Results

The solubility of phenanthrene in mixtures of carbon dioxide with toluene, acetone, or tetrahydrofuran was studied at 298 K and pressures ranging from 1.3 to 5.8 MPa. The mole fraction of carbon dioxide and phenanthrene in the liquid phase and the system pressure are shown in Table 7-1 for the three organic solvents studied. For all three systems, as more carbon dioxide is added the phenanthrene solubility decreases approaching the solubility in pure liquid carbon dioxide.

The solubility of phenanthrene as a function of system pressure, as shown in Figure 7-13, is dependent upon the organic solvent. These differences are most likely due to the differences in solubility of carbon dioxide in the pure organic solvent. For the carbon dioxide/organic binary systems, at the same pressure carbon dioxide is most soluble in acetone demonstrating slight negative deviations in activity coefficients, less soluble in tetrahydrofuran, and least soluble in toluene. This is consistent with the results for the ternary system. The solubility of phenanthrene as a function of carbon dioxide pressure changes most rapidly in acetone; for toluene as the organic solvent the solubility does not decrease rapidly until approximately 45 bar of carbon dioxide has been added.

The anti-solvent power of carbon dioxide in the solvent systems can be effectively compared by normalizing the pressure effect and considering the solubility as a function of solvent composition only. Rather than the mole fraction of carbon dioxide, the mass fraction corrects for the difference in size of the all the components thus giving a better indication of the amount in solution. If the differences in density of the components are neglected, the mass fraction is essentially equivalent to the volume fraction.

Table 7-1. Solubility of phenanthrene in CO_2 + toluene, CO_2 + acetone, and CO_2 + tetrahydrofuran mixtures at 298 K.

T (K)	Solvent	P	x^{CO2}	x^{phen}
298	Toluene	16.3	0.134	0.1684
298	Toluene	35.4	0.258	0.1553
298	Toluene	50.3	0.597	0.0604
298	Toluene	55.0	0.809	0.0128
298	Toluene	58.2	0.913	0.0034
298	Acetone	13.2	0.189	0.0890
298	Acetone	24.0	0.350	0.0500
298	Acetone	34.3	0.591	0.0222
298	Acetone	43.2	0.691	0.0111
298	Acetone	50.6	0.830	0.0044
298	Tetrahydrofuran	12.6	0.122	0.2258
298	Tetrahydrofuran	22.3	0.225	0.1857
298	Tetrahydrofuran	31.4	0.301	0.1633
298	Tetrahydrofuran	42.8	0.526	0.0903
298	Tetrahydrofuran	47.9	0.634	0.0414
298	Tetrahydrofuran	53.3	0.780	0.0107

The anti-solvent effect can be further normalized by dividing the concentration in the 3-component system by the concentration in the pure organic solvent. The normalized mass fraction ratio of phenanthrene versus the mass fraction of carbon dioxide in the three organic solvents is shown in Figure 7-6.

Carbon dioxide has the greatest effect on the solubility of phenanthrene for acetone as the organic solvent for mass fractions less than 0.60. This indicates that carbon dioxide affects the solvation of phenanthrene with a lower overall mass fraction in comparison to the other organic solvents studied. The local environment or syndiotatic region of the solute molecule is composed of a solvent mixture that may or may not be the same as the bulk concentration. For toluene and tetrahydrofuran as the organic solvent, Figure 7-6 implies that in the solvation shell the solvent molecules remain at a higher concentration than it does for acetone as the solvent for the same mass of carbon dioxide added to the system. This is a balance of forces between the interactions of the organic solvent with the solute molecule and the anti-solvent interactions with the solvent molecules. For acetone as the solvent, the more favorable interactions of carbon dioxide with acetone are significantly strong, allowing carbon dioxide to be in sufficient concentration in the syndiotactic region. For tetrahydrofuran, which has similar interactions with carbon dioxide as acetone, the favorable interactions of tetrahydrofuran with phenanthrene maintain the solvation shell and lower the local concentration of carbon dioxide around the solute molecule. Of course, at sufficiently high carbon dioxide concentrations in the bulk phase, the solvation shell becomes rich enough in carbon dioxide and the solubility decrease is similar for all the organic solvents.

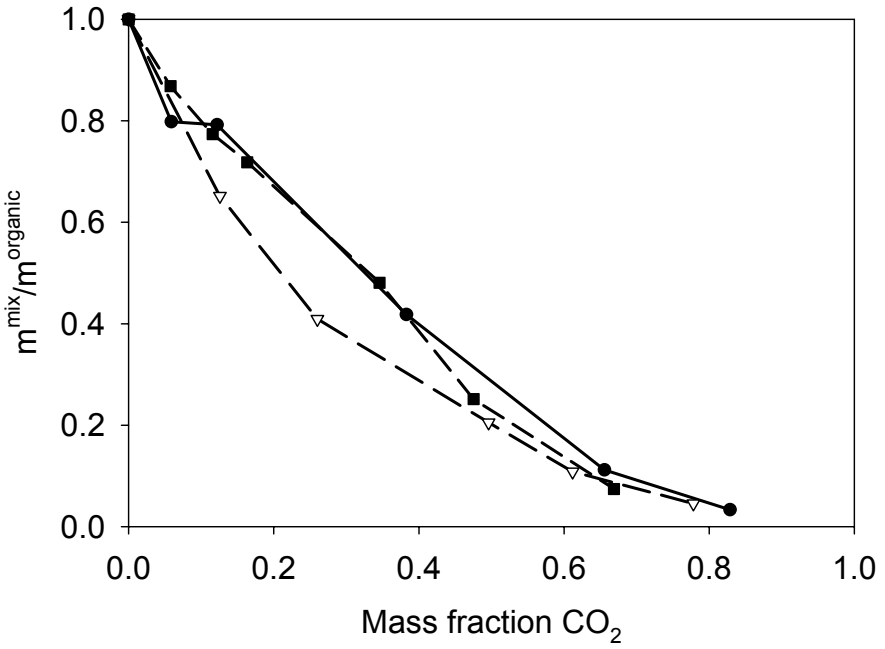


Figure 7-6. The ratio of mass fraction of phenanthrene in CO_2 + organic mixtures to phenanthrene in pure organic versus the mass fraction of CO_2. Toluene(●), acetone (▽), tetrahydrofuran (■).

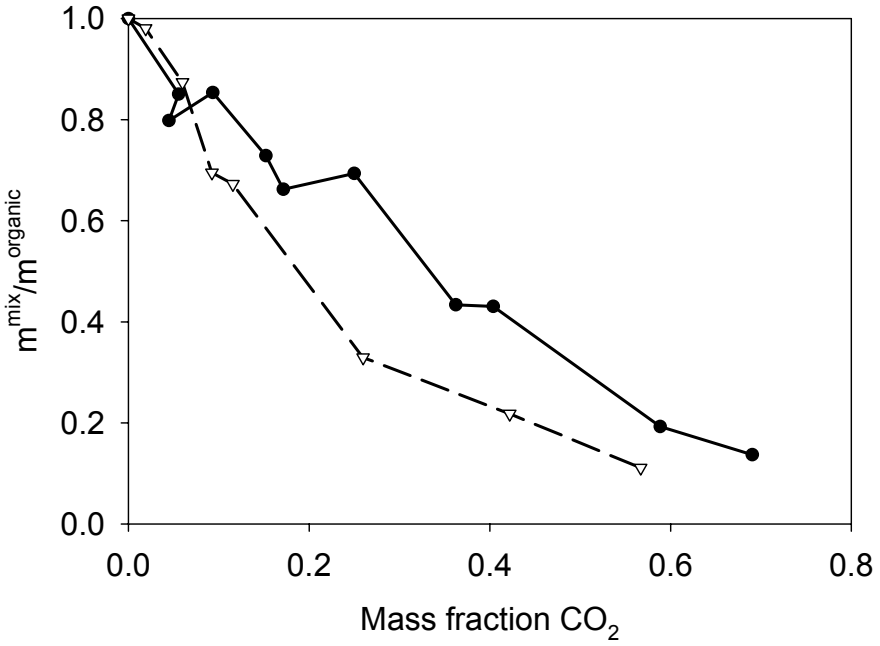


Figure 7-7. The ratio of mass fraction of acetaminophen in CO_2 + organic mixtures to phenanthrene in pure organic versus the mass fraction of CO_2. Ethanol(●), acetone (▽).

The solubility of acetaminophen in mixtures of carbon dioxide with ethanol or acetone was studied at 298 K and pressures ranging from 0.2 to 5.8 MPa. The mole fraction of carbon dioxide and acetaminophen in the liquid phase with the system pressure results are shown in Table 7-2 for both organic solvents studied. For both systems, as more carbon dioxide is added the solubility decreases approaching the solubility of acetaminophen in pure liquid carbon dioxide.

The normalized mass fraction of acetaminophen for mixtures of carbon dioxide with acetone and ethanol for the solubility of acetaminophen is shown in Figure 7-7. This difference in anti-solvent power is similar to the case of phenanthrene previously discussed. The results indicate that ethanol is able to solvate acetaminophen better than acetone in the presence of the same mass fraction of carbon dioxide in the bulk phase. This is consistent with the favorable interactions that ethanol can have with acetaminophen through hydrogen bonds; it is evident that carbon dioxide is only able to interrupt the solute-solvent interactions at high bulk concentrations.

Table 7-2. Solubility of acetaminophen in CO_2 + ethanol and CO_2 + acetone mixtures at 298 K.

T (K)	Solvent	P	x^{CO2}	x^{phen}
298	Ethanol	7.0	0.065	0.0415
298	Ethanol	9.9	0.052	0.0387
298	Ethanol	17.0	0.109	0.0416
298	Ethanol	20.2	0.174	0.0348
298	Ethanol	30.3	0.194	0.0313
298	Ethanol	37.9	0.283	0.0328
298	Ethanol	48.8	0.394	0.0197
298	Ethanol	50.3	0.438	0.0195
298	Ethanol	55.4	0.614	0.0084
298	Ethanol	57.9	0.712	0.0059
298	Acetone	2.3	0.027	0.0389
298	Acetone	4.3	0.083	0.0339
298	Acetone	6.6	0.125	0.0263
298	Acetone	10.1	0.155	0.0252
298	Acetone	17.6	0.324	0.0115
298	Acetone	27.0	0.498	0.0072
298	Acetone	37.0	0.638	0.0035

Thermodynamic Modeling

In Chapter II the MOSCED model was shown to be successful at correlating parameters for multifunctional solid compounds and predicting the solubility in a variety of pure organic solvent and mixtures of organic solvents. Additionally, the MOSCED model was able to successfully correlate Henry's constants in organic solvents for several gases including carbon dioxide. The capabilities of the MOSCED model to predict solid solubilities in mixed solvents consisting of organic solvents with carbon dioxide at high pressures will be evaluated. All pure component parameters have been regressed from low pressure solubility data in binary systems. The MOSCED model requires no binary or ternary interaction parameters to predict the solubility in mixed solvents.

Because the MOSCED model only predicts the activity coefficient at infinite dilution the activity coefficient must be extrapolated to finite composition and for high pressure systems to the pressure of interest. A cubic equation of state, such as the Peng-Robinson with Gibbs free energy based mixing rules, as discussed in Chapter VI, is a favorable technique to use in conjunction with the MOSCED model. The binary interaction parameters for the free energy model can be calculated from the predicted limiting activity coefficients of MOSCED and then applied to mixing rules such as the Huron-Vidal or Wong-Sandler.

The governing equations for the equation of state method to satisfy equilibrium fugacity for solid, liquid, and vapor phases are represented by equations 8-1 to 8-3,

$$x_1 \phi_1^L P = y_1 \hat{\phi}_1^V P \qquad \text{Eq. 8-1}$$

$$x_2\phi_2^L P = y_2\hat{\phi}_2^V P \qquad \text{Eq. 8-2}$$

$$P_3^{sub}\exp\left[\frac{v^S P}{RT}\right] = x_3\phi_3^L P \qquad \text{Eq. 8-3}$$

where P is pressure, x_i is the mole fraction in the liquid phase, y_i is the mole fraction in the vapor phase, ϕ_i^L and ϕ_i^V are the fugacity coefficients in the liquid phase and vapor phase respectively, P^{sub} and v^S are the sublimation pressure and molar volume of the solid component. The most useful cubic equations of state use the corresponding states principle to calculate the pure component parameters. This requires knowledge of the critical properties of all components to calculate the necessary EoS parameters. For multifunctional compounds the critical properties are generally not known, especially if they have only been recently synthesized, and even for the common pharmaceutical acetaminophen, the critical properties have not been measured. This limits the general applicability of this approach to predicting the composition of solids in high pressure mixed solvent systems.

The use of a liquid activity coefficient model for the liquid phase eliminates the need to know the critical properties of the solid component. This method, often referred to as the γ–ϕ method, can be used very easily with the activity coefficients of the MOSCED model. As before the predicted limiting activity coefficients are used to calculate the interaction parameters for an activity coefficient model, such as NRTL or UNIQUAC. The pressure correction to the activity coefficient is calculated using the Poynting correction. For the two volatile components, carbon dioxide and the organic,

the governing equilibrium equations are represented by equation 8-4 and 8-5. For the solid phase the ideal solubility calculated from the pure solid enthalpy of fusion, melting point, and heat capacity must be equal to the activity of the solid in the liquid phase mixture, as shown in equation 8-6.

$$x_1\gamma_1 \exp\left[\int_1^P \frac{\bar{v}_1^{\,L}}{RT}dP\right]\phi_1^{sat}P_1^{sat}\exp\left[\int_{P^{sat}}^1 \frac{v_1^{\,L}}{RT}dP\right] = y_1\hat{\phi}_1 P \qquad \text{Eq. 8-4}$$

$$x_2\gamma_2 \exp\left[\int_1^P \frac{\bar{v}_2^{\,L}}{RT}dP\right]\phi_2^{sat}P_2^{sat}\exp\left[\int_{P^{sat}}^1 \frac{v_2^{\,L}}{RT}dP\right] = y_2\hat{\phi}_2 P \qquad \text{Eq. 8-5}$$

$$x_3\gamma_3 = x_3^{\,ideal} = \exp\left[\frac{-\Delta H_{fus}}{RT_m}\left(\frac{T_m}{T}-1\right)-\frac{\Delta C_p}{R}\left(\ln\frac{T_m}{T}-\frac{T_m}{T}+1\right)\right] \qquad \text{Eq. 8-6}$$

For the volatile components the partial molar volume is assumed equivalent to the liquid molar volume. The three unknown variables are x_1, x_2, and P.

Before attempting the prediction of the ternary system, the phase behavior of the constituent binary systems is predicted. The VLE of carbon dioxide in all the organic solvents used in this study are predicted an compared to literature data. The prediction of the solubility of the solids in carbon dioxide is also predicted and compared to literature values.

Prediction of CO_2 + organic VLE

For the prediction of the two-component VLE there are two approaches available as discussed already, an EoS with gE based mixing rules or the γ–ϕ method. For the EoS

method there are several applicable mixing rules available, Huron-Vidal, Modified Huron-Vidal 1 (MHV1), Modified Huron-Vidal 2 (MHV2), Huron-Vidal-Orbey-Sandler (HVOS), and Wong-Sandler (WS), with all the pertinent equations shown in Appendix A. The Wong-Sandler mixing rule will not be examined because of the extra fitting parameter that cannot be predicted using the MOSCED model.

Comparing the predictions for the mixing rules for the example system of carbon dioxide + toluene, it can be seen from Figure 7-8 that all mixing rules with the exception of the Huron-Vidal rule terribly under-predict the solubility of CO_2 in the liquid phase. The MOSCED model predicts for the binary system limiting activity coefficients for CO_2 in toluene $\gamma^{\infty} = 2.02$ and for toluene in CO_2 $\gamma^{\infty} = 6.83$. All the mixing rules, including HV, predict much larger infinite dilution activity coefficients, on the order of 1000 for CO_2 in toluene. This difference in activity coefficient is assumed to be due to the difference in reference state of the activity coefficient model which is always referenced at 0 bar and the equation of state which is referenced to the pressure of interest.

The differences in performance of the mixing rules may be due to the differences in reference pressure of the difference models. The HVOS, MHV1, and MHV2 calculate the excess Gibbs free energy and activity coefficients at a low pressure, so that available low pressure interaction parameters can be used directly into the equation of state. The HV rule calculates the excess free energy at an infinite pressure reference state, thus making interaction parameters calculated at low pressure not directly applicable to the EoS. The MOSCED model uses a reference pressure of 0 bar, assuming carbon dioxide is in a hypothetical liquid state. In correlating the Henry's constants of carbon dioxide,

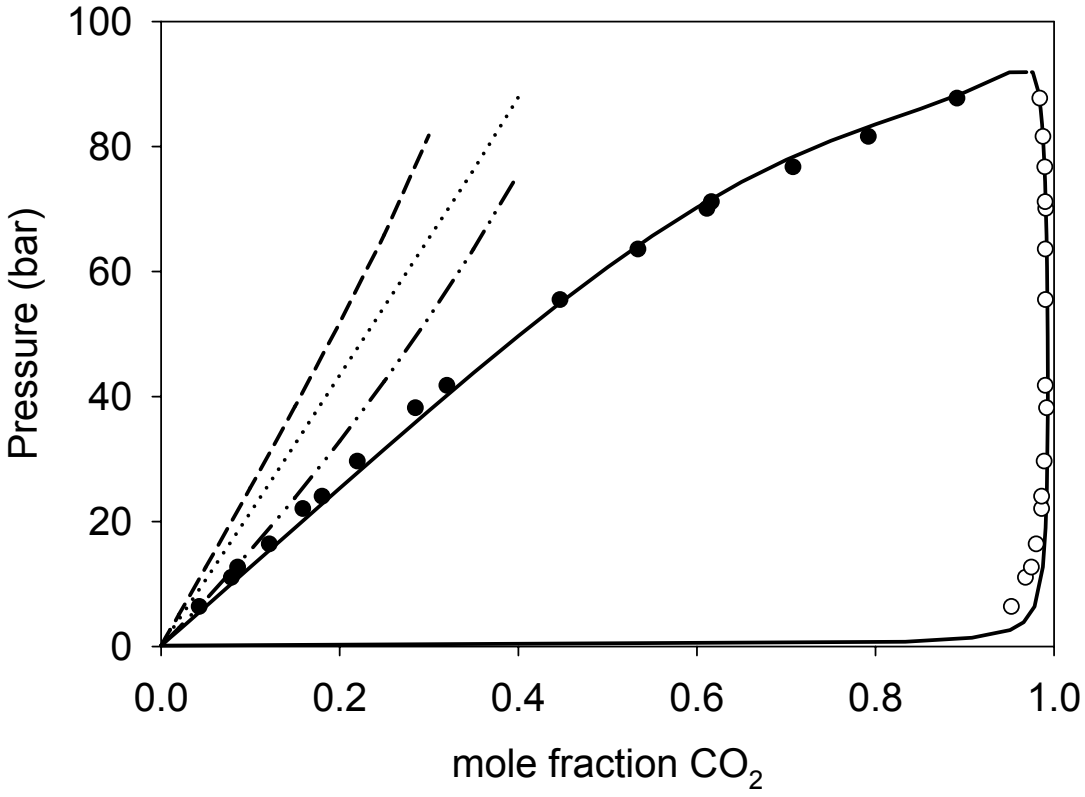


Figure 7-8. VLE of toluene + carbon dioxide at 323 K(●,○)(Fink and Hershey 1990). Lines are predictions using PRSV EoS and MOSCED/UNIQUAC with HV (——), HVOS (– – –), MHV1 (.....), MHV2 (— . . —) mixing rules.

the hypothetical liquid fugacity of CO_2 at 0 bar is found from extrapolating the fugacity pressures above the vapor pressure or for temperatures above the critical temperature the fugacity is extrapolated from the linear region at high pressures. While the reference pressures for 0 bar mixing rules and MOSCED parameters match, the infinite pressure referenced mixing rule proves to give a better prediction. For the zero pressure reference mixing rules, it is not explicit that the carbon dioxide is in the hypothetical liquid state, whereas with the infinite pressure reference the gas would necessarily remain in the liquid state. This error with the 0 bar mixing rules may be due some errors in the implicit extrapolation to the hypothetical liquid state. Because the parameters for CO_2 were correlated to only data for CO_2 as a solute, the prediction of MOSCED for the other side, CO_2 as a solvent may not be as reliable for prediction. The equation of state mixing rules prove to be equally sensitive to both limiting activity coefficient values used to calculate interaction parameters; this may contribute to the error in predictions with this technique.

Predictions using the γ–ϕ method remove the uncertainties in the reference pressures associated with the use of equations of state. The predictions of the binary carbon dioxide + organic systems using this method are shown in Figures 7 through 10. For all four systems considered here, the predictions agree very well with the literature *P-x-y* data. The model tends to give higher pressures than the literature data, but is able to predict both the slight negative deviations from ideality in the acetone system (Figure 7-10) and the positive deviations in the case of toluene (Figure 7-9) and ethanol (Figure 7-

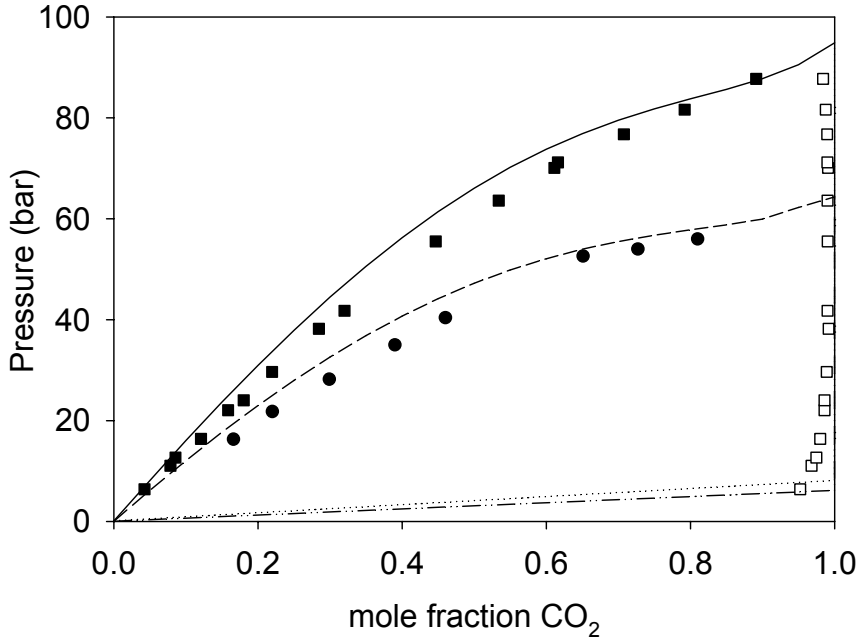


Figure 7-9. VLE of toluene + carbon dioxide at 298 K(●)(Chang 1992) and 323 K(■,□)(Fink 1990). Lines are predictions using MOSCED with UNIQUAC.

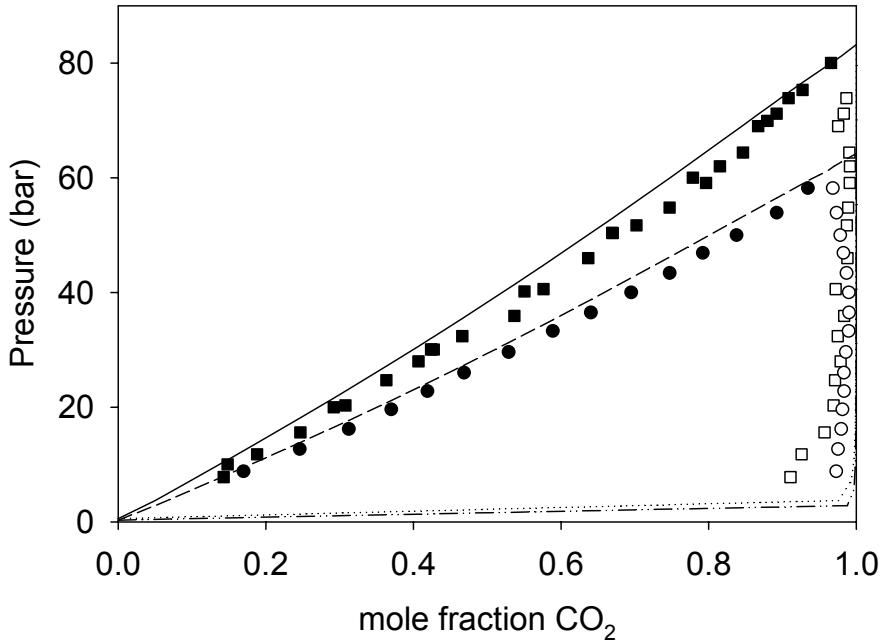


Figure 7-10. VLE of acetone + carbon dioxide at 298 K(●,○)(Chang 1998)and 313 K(■,□)(Chang 1998) (Adrian 1997). Lines are predictions using MOSCED with UNIQUAC.

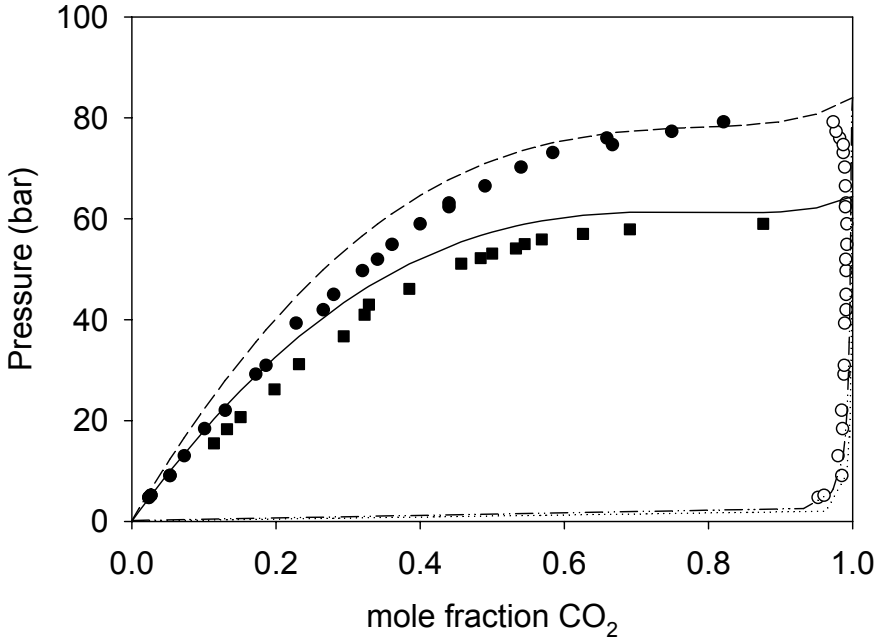


Figure 7-11. VLE of ethanol + carbon dioxide at 298 K(■)(Kordikowski 1995) and 313 K(●,○)(Galacia-Luna 2000) (Chang 1998). Lines are predictions using MOSCED with UNIQUAC.

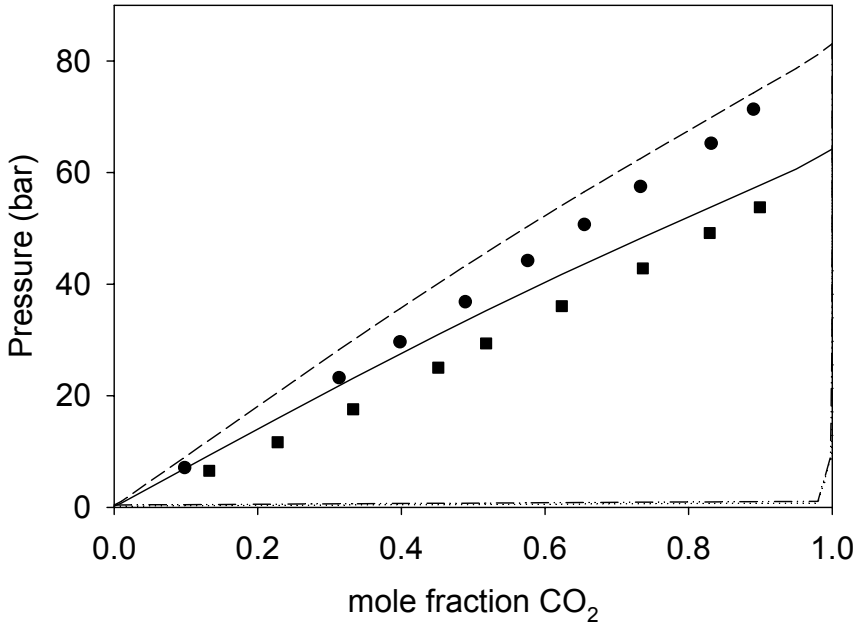


Figure 7-12. VLE of tetrahydrofuran + carbon dioxide at 298 K(●,○) and 313 K(■,□) (see Chapter IV). Lines are predictions using MOSCED with UNIQUAC.

11). The MOSCED model performs poorest for the THF system, predicting slight positive deviations, whereas the system demonstrates nearly ideal solution behavior. While this method may not be as quantitative as the EoS method with HV mixing rules, it does not require any critical properties and is generally applicable to any system where the MOSCED parameters are known.

Prediction of solid solubility in sc-CO_2

Use of the γ–ϕ method here requires the use of an equation of state to calculate the partial molar volume of the solute in the liquid phase to account for pressure dependency of the activity coefficient. This molar volume is known to be a strong function of pressure for solutes in a supercritical fluid and can be calculated using an equation of state. Since an EoS is necessary to calculate the partial molar volume the EoS is used to calculate the solution non-ideality. The same approach is used as discussed previously. For these predictions the Peng-Robinson EoS is used with the Huron-Vidal mixing rules with UNIQUAC g^E model. No significant difference was found between the NRTL or UNIQUAC g^E models in this study.

The solubility of phenathrene in carbon dioxide at several temperatures as a function of CO2 density are shown in Figure 7-13 along with the model predictions. The predictions match the general trend of the data, with a tendency to over-predict the solubility at the lowest temperature studied of 308 K. The inaccurate predictions could be attributed to the inability of the equation of state to accurately model the P-V-T

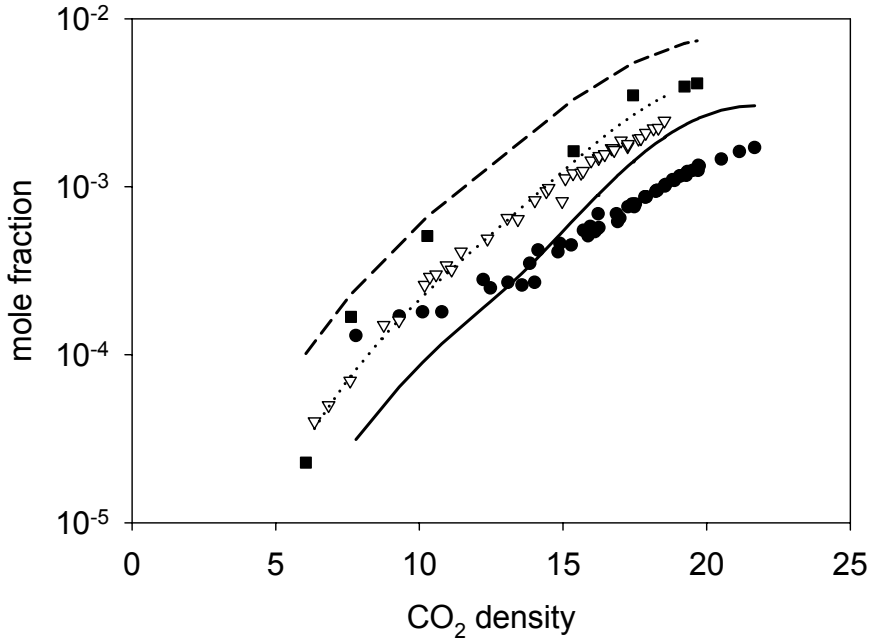


Figure 7-13. Solubility of phenanthrene in sc-CO_2 at 308 K(●)(Dobbs 1986; Bartle 1990), 323 K(▽)(Bartle 1990) and 343 K(■)(Johnston 1982). Lines are predictions using MOSCED with PRSV-HV-UNIQUAC.

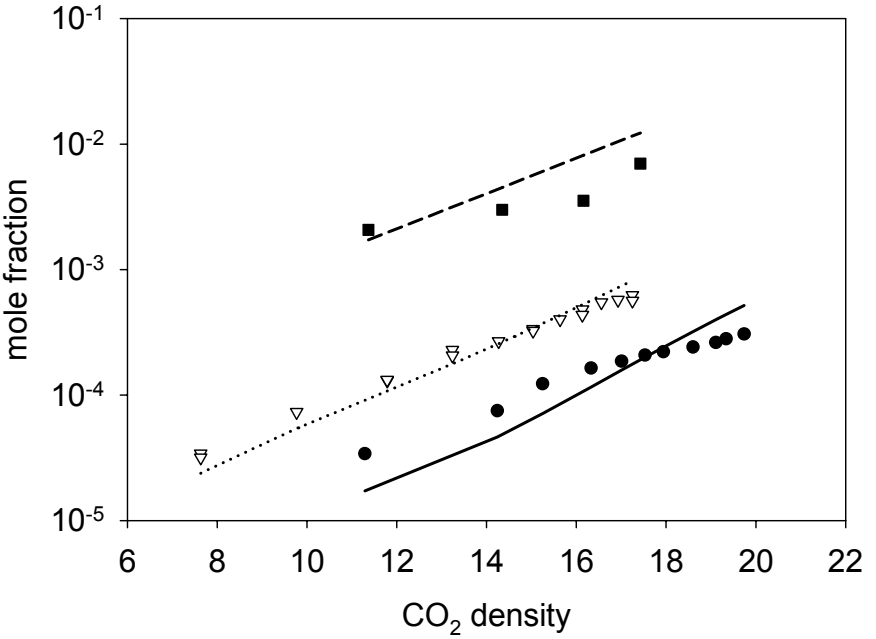


Figure 7-14. Solubility of o-hydroxybenzoic acid at 308 K(●) (Gurdial 1991), 328 K(▽) (Gurdial 1991; Lucien 1996) and 373 K(■) (Krukonis 1985). Lines are predictions using MOSCED with PRSV-HV-UNIQUAC.

properties of the pure carbon dioxide at a temperature so near to the critical temperature of 304 K and not to the MOSCED activity coefficient predictions.

The solubility of acetaminophen in carbon dioxide over a temperature and pressure range is not available in the literature, but data for o-hydroxybenzoic acid, a compound of similar structure and functionality, are available. As shown in Figure 7-14, the model matches the literature data very well for the broad temperature range of 308 to 373 K.

A comparison of the various g^E based mixing rules for the supercritical carbon dioxide systems are shown in Figure 7-15. The MHV1, MHV2, and HVOS models under-predict the solubility of phenanthrene in carbon dioxide at 308 K. This is similar to the under-prediction of the solubility of carbon dioxide in toluene discussed earlier, and the same arguments apply here. The good prediction of the HV model does however validate the MOSCED parameter for carbon dioxide being appropriate for predicting systems where carbon dioxide is the solvent or dominant component.

Prediction of solid solubility in CO_2-expanded liquids

The MOSCED model has been shown capable of predicting the phase behavior of the binary systems of carbon dioxide + organic solvent and solid + carbon dioxide. The γ–ϕ method with UNIQUAC as the activity coefficient model will be used to extend the prediction to the ternary systems of carbon dioxide + organic + solid and compared to the experimentally determined data. The UNIQUAC activity coefficient model will be used to extrapolate the infinite dilution activity coefficients to finite concentrations.

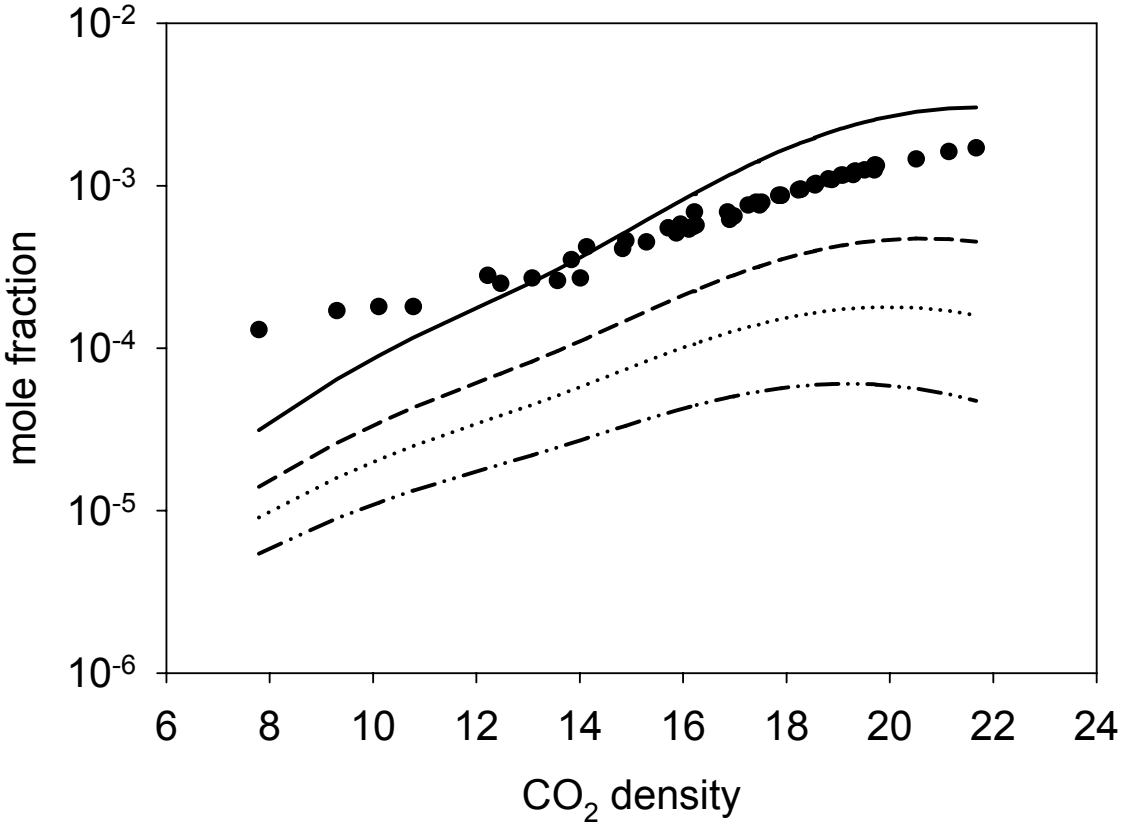


Figure 7-15. Solubility of phenanthrene in sc-CO_2 at 308 K(●) (Dobbs, Wong et al. 1986; Bartle, Clifford et al. 1990). Lines are predictions using MOSCED with PRSV and various mixing rules. HV (——), MHV2 (– – –), HVOS (.....), MHV1 (— . . —).

The predictions of the solubility of phenanthrene at 298 K as a function of pressure in the mixtures carbon dioxide with three different organic solvents are shown in Figure 7-16. For acetone and tetrahydrofuran, the model predicts the solubility as a function of carbon dioxide pressure very well. The model over-predicts the solubility of phenanthrene for toluene as the solvent, predicting a drastic decrease in solubility at approximately 58 bar that is not in agreement with experimental data. The solubility of phenanthrene in pure liquid carbon dioxide is also over-predicted by an order of magnitude. This indicates that the MOSCED model is not predicting a sufficiently large activity coefficient at infinite dilution; this may also account for the failure of the model to predict correctly the composition dependency in the toluene system.

The predictions of the solubility of acetaminophen at 298 K as a function of pressure in mixtures of carbon dioxide with acetone or ethanol are shown in Figure 7-17. The model correctly predicts the solubility in the carbon dioxide expanded ethanol, capturing the tremendous decrease in solubility at around 60 bar CO_2 pressure. The MOSCED model underpredicts the solubility of acetaminophen in pure acetone. This causes the under-prediction in the mixed solvent, although the shape of the curve matches the trend of the experimental data. The model predicts the solubility in pure carbon dioxide at around 5×10^{-6}. Considering the structure of acetaminophen, this estimation of solubility is reasonable and consistent with the solubility of o-hydroxybenzoic acid as discussed previously. In general the MOSCED model is able to predict the infinite dilution activity coefficients of the solid in the pure liquids and the UNIQUAC model is able to successfully extrapolate the activity coefficients to finite concentrations.

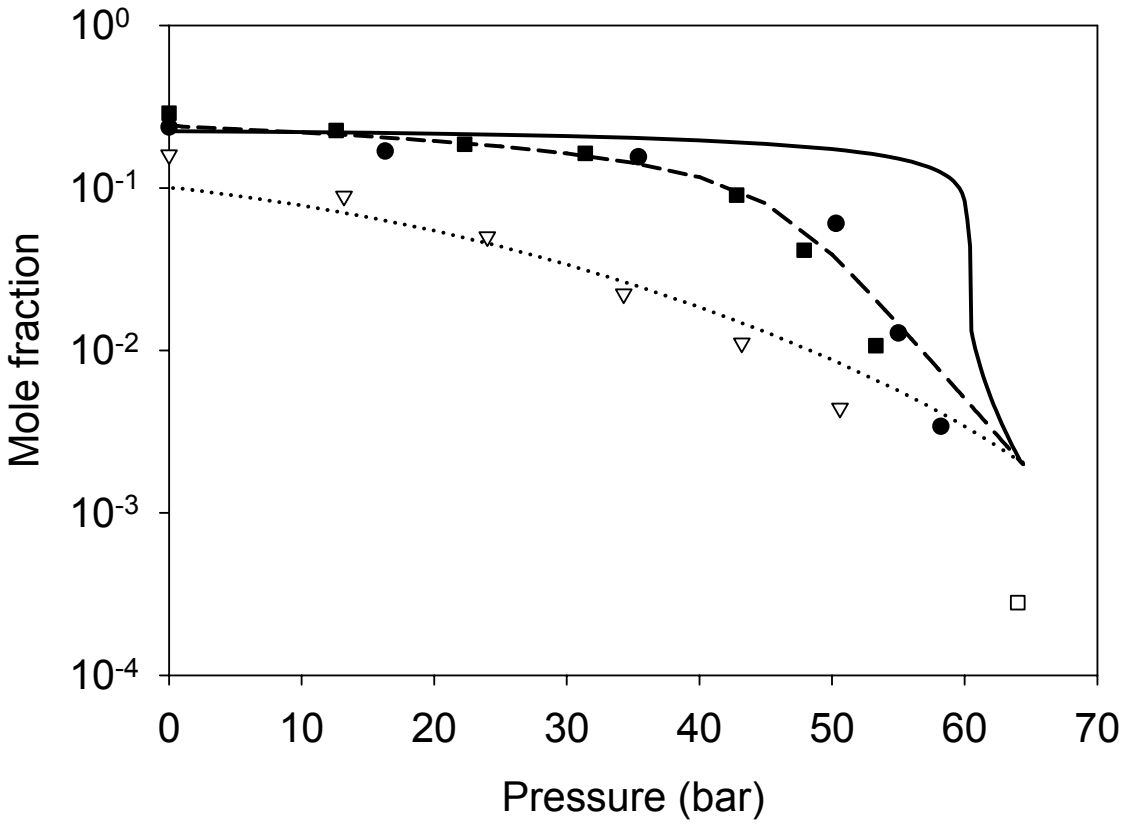


Figure 7-16. Solubility of phenanthrene at 298 K in mixtures of carbon dioxide with toluene (●), acetone (▽),and tetrahydrofuran (■). Predictions using MOSCED with UNIQUAC. Toluene (_____), acetone (.....), and tetrahydrofuran (_ _ _).

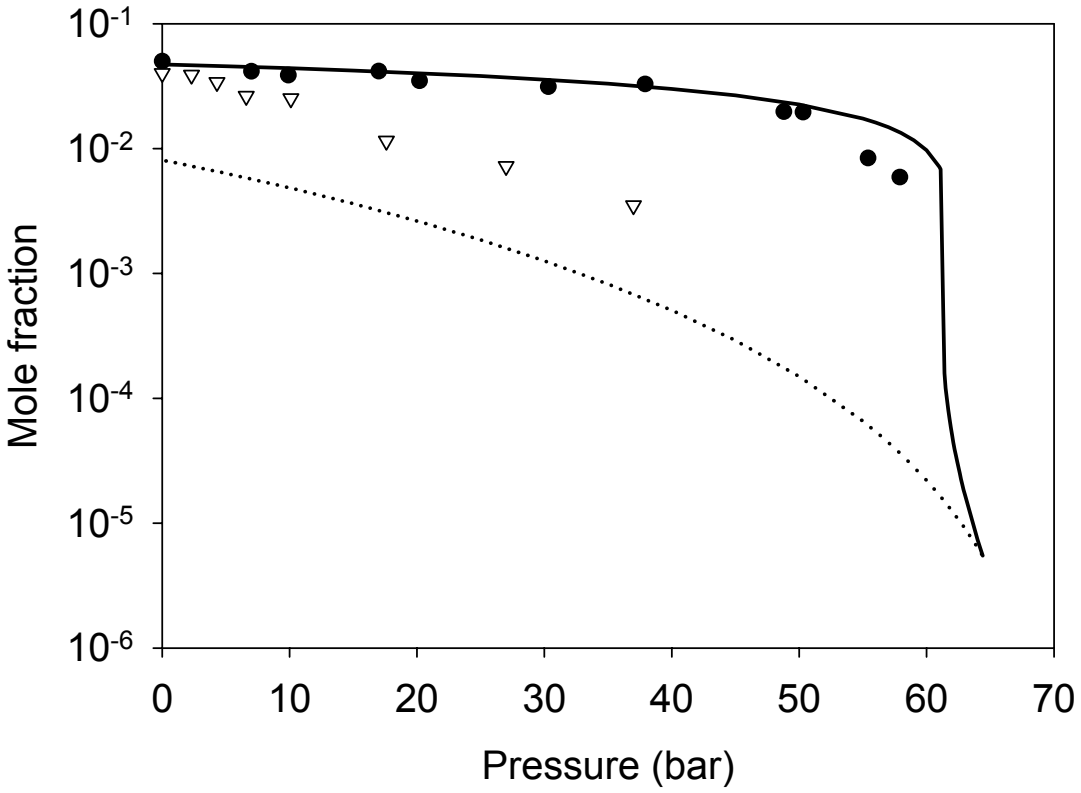


Figure 7-17. Solubility of acetaminophen at 298 K in mixtures of carbon dioxide with ethanol (●) and acetone (▽). Predictions using MOSCED with UNIQUAC. Ethanol (——), acetone (.....).

Comparison of CO_2 and hexane as an anti-solvent

The solubility of acetaminophen is very low in hexane as well as in liquid carbon dioxide, as already demonstrated. Hexane therefore, would serve as a suitable anti-solvent for the crystallization of acetaminophen. The effectiveness of carbon dioxide as an anti-solvent has already been demonstrated and effectively predicted by the MOSCED model. The solubility of acetaminophen in mixtures of ethanol + hexane is also examined and the phase behavior is predicted.

The solubility of acetaminophen in mixtures of ethanol + hexane at 298 K are shown in Table 7-3. Compositions of the equilibrium liquid are given both as the total composition and the composition of the liquid solvent is also given on a solute free basis. In terms of mole fraction solubility, hexane proves to be a better anti-solvent, resulting in a lower solubility for the same solvent mole fraction, as seen in Figure 7-18.

There no specific interactions, i.e. hydrogen bonds or dipole-dipole, that a straight chain alkane, in this case hexane, can have with acetaminophen. However, carbon dioxide can act as Lewis acid in solution, as discussed previously in Chapter IV, and could potentially be specifically interacting with the solute. The molecular weight disparity between hexane and carbon dioxide is also contributing to the solubility differences because per mole hexane is able to displace more area. Considering the solubility of acetaminophen on a mass fraction basis normalizes the size difference and makes a direct comparison possible between the two anti-solvents. As shown in Figure 7-19, the mass fraction solubility of acetaminophen as a function of anti-solvent mass fraction for both hexane and carbon dioxide are very similar. This implies there is no

Table 7-3. Solubility of acetaminophen in mixtures of ethanol and hexane at 298 K. Composition shown in mole fraction, x, and mass fraction m. The solvent composition for mass fraction is given on a solute free basis.

Total composition			Solute free		
x^{EtOH}	x^{Hex}	x^{Phen}	m^{EtOH}	m^{Hex}	m^{Phen}
0.9500	0.0000	0.0500	1.0000	0.0000	0.1916
0.9190	0.0380	0.0430	0.9282	0.0718	0.1634
0.8931	0.0689	0.0380	0.8738	0.1262	0.1434
0.8617	0.1074	0.0310	0.8109	0.1891	0.1160
0.7924	0.1871	0.0250	0.6936	0.3064	0.0747
0.7799	0.1999	0.0202	0.6759	0.3241	0.0732
0.7481	0.2357	0.0162	0.6292	0.3708	0.0579
0.5468	0.4423	0.0109	0.3979	0.6021	0.0345
0.3556	0.6421	0.0023	0.2284	0.7716	0.0067
0.2345	0.7648	0.0008	0.1408	0.8592	0.0021

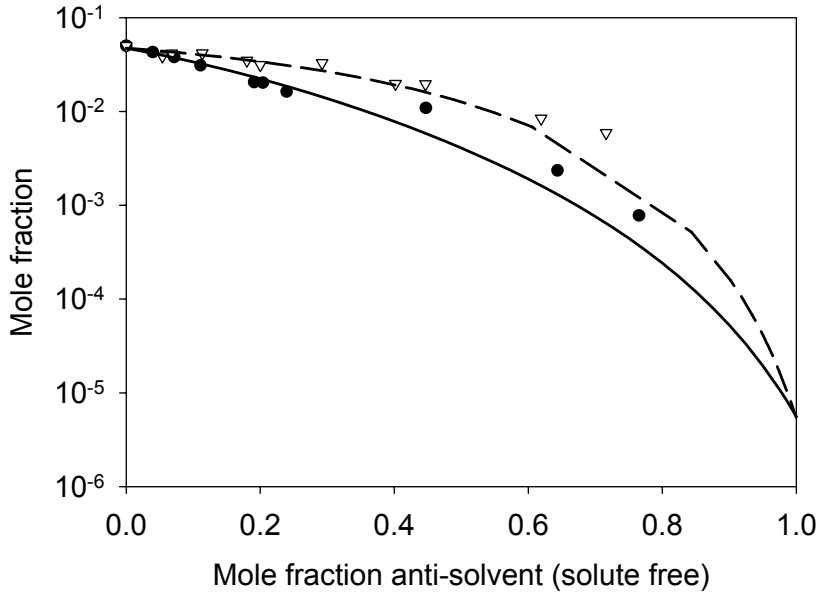


Figure 7-18. Comparison of anti-solvents. Solubility of acetaminophen at 298 K in mixtures of ethanol with hexane (●) and carbon dioxide (▽). Predictions using MOSCED with UNIQUAC. Hexane (——), CO_2 (– – –).

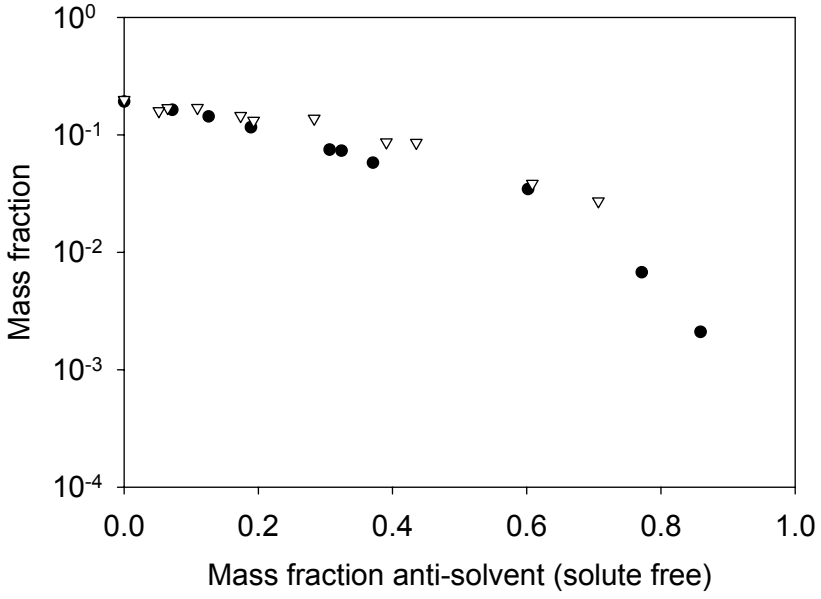


Figure 7-19. Comparison of anti-solvents by mass fraction. Mass fraction solubility of acetaminophen at 298 K in mixtures of ethanol with hexane (●) and carbon dioxide (▽).

difference between the interactions of acetaminophen with carbon dioxide or hexane and the solubility differences are only due to the size differences of the anti-solvent.

Although hexane proves to be an equivalent anti-solvent to carbon dioxide the processing involved for the two solvents are different. An idealized process for the crystallization of acetaminophen from ethanol with hexane would involve the distillation of the mixed process solvent to separate the hexane from the mixed solvent. Alternatively, a depressurization step is all that is necessary to separate the carbon dioxide from the mixed solvent. However this does introduce the added cost of cooling/compressing the carbon dioxide to cause the desired solubility of the solute in the liquid phase. A comparison of the most cost efficient process would ultimately come down to the distillation costs for the hexane process and the pressurization costs for the carbon dioxide process.

Summary

Several solvent systems for the anti-solvent processing of solid compounds have been investigated. The solubility of a poly-aromatic solid compound, phenanthrene, has been measured in mixtures of toluene, acetone, or tetrahydrofuran with carbon dioxide at 298 K; additionally, the solubility of a functionalized solid compound, acetaminophen, has been measured in mixtures of ethanol or acetone with carbon dioxide at 298K. The predominant effect of solubility in the carbon dioxide expanded solvent has been shown to be the interaction of the organic solvent with carbon dioxide. A comparison of carbon dioxide with hexane as anti-solvents in the binary system of ethanol + acetaminophen

implied there is little difference in the interactions of carbon dioxide or hexane with acetaminophen.

All phase behavior of all the solvent systems were successfully predicted using the MOSCED model. The predicted binary infinite dilution activity coefficients calculated only from pure component parameters were able to successfully correlate the VLE of the carbon dioxide + organic solvent systems, the solid solubility in super-critical carbon dioxide, and the solid solubility in the carbon dioxide expanded liquid.

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CHAPTER VIII

FINAL SUMMARY AND RECOMMENDATIONS

This work has focused on identifying solvents and solvent mixtures useful for reactions and separations. Prediction of solution thermodynamic properties can reduce experimental effort and allow for easy identification of solvent mixtures that may offer an advantage over pure solvents. A modified cohesive energy density model was used to predict the solid-liquid-equilibria for multifunctional solids in pure and mixed solvents for identification of solvents for design of crystallization processes.

Replacement of traditional organic solvents with environmentally benign alternatives was also investigated. Carbon dioxide is an ideal solvent alternative because of its miscibility with many organic solvents, non-toxicity, and environmental benignity. The high pressure vapor-liquid equilibria of mixed solvents of carbon dioxide and organic liquids were studied with potential use as reaction solvents, where the pressure tunable properties of the solvent mixture can be manipulated to optimize reaction conditions. Applications of gas-expanded liquids to the anti-solvent crystallization of some model pharmaceuticals were also investigated.

The low solubility of carbon dioxide in water has been exploited to develop novel solvent mixtures to extend water/organic biphasic catalytic systems to include a carbon dioxide induced immiscibility for the immobilization of homogeneous catalysts. This

avoids interphase the mass transfer limitations, allowing for reaction in a single homogeneous phase, and facile catalyst sequestration with minimal pressures of carbon dioxide added.

MOSCED model

A database of limiting activity coefficient data available in the literature were collected and used to reexamine the MOSCED model. The model has been shown in correlate liquid activity coefficient data to an average deviation of 10.6%, including data for water as a solvent. The model successfully predicted the limiting activity coefficients for multifunctional solid compounds of interest to the pharmaceutical/agricultural industry with an average deviation in solubility of 24% for the 26 solid compounds studied compared to a 39% deviation for 15 of the solids with the UNIFAC model that have available parameters. A technique for measurement of solid solubilities in pure and mixed organic solvents was developed and used to further test the capabilities of the MOSCED model. Additionally the model was able to predict the solubility of solid compounds in mixed solvents including those of carbon dioxide and organic liquids with some success.

Many pharmaceutical compounds include ionic pairs to increase water solubility and bioavailability and many are tightly bound with water often occurring as hydrates of water. Some modification of the model is necessary to include the longer range forces present with ionic interactions, and make it generally applicable to any solute-solvent system. If the excess Gibbs free energy is divided into the sum of short range forces (i.e.

dispersion) and longer range coulombic forces that may accounted for by the Debye-Hückel expression (Robinson and Stokes 1970) for activity of the electrostatic interaction, as shown in equation 8-1. While this expression is more correct for dilute

$$\ln \gamma_i = -\left(\frac{e^2}{\varepsilon_0 \varepsilon_r RT} \right)^{3/2} \frac{N_A^{\ 2}}{8\pi} (2d_s)^{1/2} |z_+ z_-| I^{1/2} \qquad \text{Eq. 8-1}$$

solutions of electrolytes, extension of the limiting activity coefficients to finite concentrations will necessarily include the effect of ion-ion interactions and incomplete dissociation or ion pairing. The several modified NRTL models (Cruz and Renon 1978; Chen and Evans 1986) attempt to account for these interactions, and also the model of Pitzer (Pitzer 1991) has been used successfully for describing electrolyte systems.

The MOSCED model may also be extended to the prediction of the activity of polymer solutions. This may be most directly achieved by using the enthalpic portion of the MOSCED model to calculate the interaction parameter (χ_{12}) of the Flory-Huggins theory, as is similarly done with the Hansen model (Hansen 2000). Also, the interaction parameters may be calculated to match the infinite dilution activity coefficients for a lattice-fluid equation of state like that of Sanchez and Lacombe (Sanchez and Lacombe 1976), or for hard sphere chain models, like SAFT (statistical associating fluid theory) (Chapman, Gubbins et al. 1989) or PHSC (perturbed hard-sphere-chain) (Song, Lambert et al. 1994) equations of state.

High Pressure VLE

Replacement of organic solvents as medium for reaction and separation with carbon dioxide has received much attention because of the non-toxicity, non-flammability and environmental advantages with potential decrease in VOC emissions. Mixed solvents of carbon dioxide with organic solvents have applications in anti-solvent crystallization processes and as solvents for homogeneously and heterogeneously catalyzed reactions, and for optimization of the solvent system and operating conditions knowledge of the phase behavior is required. A technique for the rapid and facile determination high pressure binary vapor-liquid-equilibria, liquid phase density and volume expansion has been developed and applied to several carbon dioxide + organic binary systems. The results reveal the unique behavior of carbon dioxide in solution, indicating that it acts as a low dispersion, slightly polar, and Lewis acidic compound.

Some preliminary results for the prediction of the carbon dioxide-organic phase behavior with the MOSCED model have been presented. The prediction of vapor-liquid equilibria is most promising using equations of state with g^E based mixing rules. Some different assumption may be necessary to make the MOSCED predictions compatible with the references assumed by the available mixing rules.

High Pressure VLLE

A novel solvent system for the sequestration of water soluble homogeneous catalysts was investigated. The addition of a polar organic solvent to an aqueous phase will enhance the solubility of the hydrophobic reactant and upon addition of carbon

dioxide two liquid phase are formed: a relatively pure water phase where the catalyst will predominantly reside, and an organic phase where the product favorably partitions. A variable volume view cell with a synthetic technique for measuring the high pressure vapor-liquid-liquid equilibria was employed for several polar organic solvents with water and carbon dioxide. While the hydroformylation of octene to nonanal is currently being explored by other researchers (Jones, Lu et al. 2004), there are other water/organic biphasic reactions that may benefit from a single solvent phase offered by this solvent system.

Other potential applications for this solvent system include the recycle of enzymes, as demonstrated by Lu and coworkers (Lu, Lazzaroni et al. 2004). However, the choice of carbon dioxide to cause the phase split may have negative effects on the activity of the enzyme as carbon dioxide acts as a sour gas through the formation of carbonic acid and thus lowering the pH of the water. Other compressible fluids with accessible critical points, like ethylene or ethane, may also be able to cause a similar phase split.

Carbon dioxide has the potential for causing a phase split with other solvent systems including polyethylene glycol (PEG), which is miscible with many polar organic solvents. The lower solubility of carbon dioxide in PEG relative to other organic compounds should result in the formation of two liquid phases. A comparison of the P-x-y diagrams for CO_2 with PEG and acetone (Figure 8-1) reveal the markedly lower solubility of carbon dioxide in liquid PEG than acetone at the same total pressure. We would expect that mixing the two liquids of CO_2 saturated acetone and CO_2 saturated

PEG at 60 bar for example, would result in the formation of two partially miscible phases because of the higher solubility of CO_2 in the acetone and thus a greater reduction in polarity. The partitioning of PEG soluble catalysts may improve because of lower solubility of PEG in the organic rich phase although pressure requirements to effect a separation may be higher than the water/organic biphasic systems.

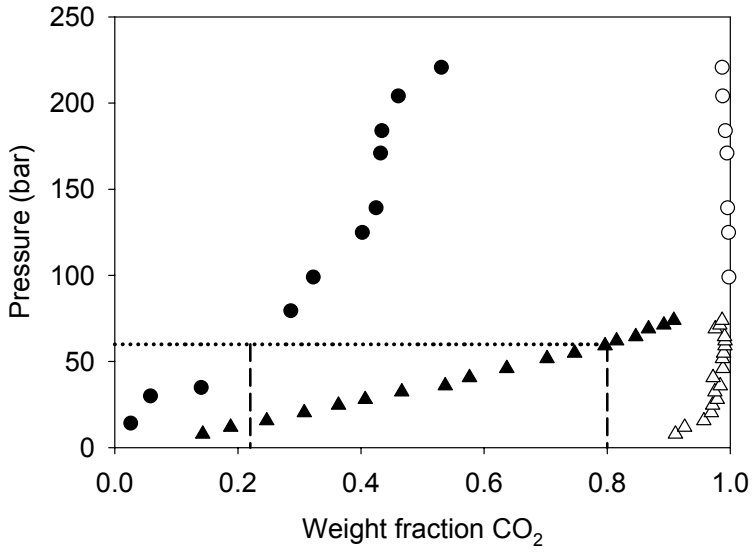

Figure 8-1. Weight fraction of CO_2 in PEG(400) (●,○)(Daneshvar, Kim et al. 1990) and acetone (▲,△)(Chang, Chiu et al. 1998) at 313 K. Dotted line with hatched line showing the composition of the liquid phase at 60 bar.

The recently proposed compressed anti-solvent precipitation and photopolymerization (CAPP) process has been applied to the polymerization of PEG1000 diacrylate in dichloromethane (Owens, Anseth et al. 2002; Owens, Anseth et al. 2003). This technique combines a polymerization reaction with the precipitation of the polymer. An understanding of the phase behavior of the multicomponent mixture of photoinitiatior, monomer, solvent, and anti-solvent will be necessary to identify the optimum reaction

conditions and serve as a template for extension of the process to other reacting systems. Combining the reaction and precipitation for other organic products may prove useful in controlling morphology and size of the precipitate, although the applicable reactions have not yet been identified.

The formation of a solid phase at 15 °C and less than 30 bar in the carbon dioxide + tetrahydrofuran + water system may have potential applications to the sequestration of carbon dioxide from flue gas. The tetrahydrofuran is known to form clathrate-hydrates at at around 4 °C at a around a 17: 1 (H2O:THF) mole ratio, and the addition of carbon dioxide raises the temperature of clathrate formation. Assuming a large portion of carbon dioxide is incorporated into the solid phase, the system could be used to remove carbon dioxide from the gaseous emissions of power plants at a low energy cost, and disposed of in the deep ocean (Takano, Yamasaki et al. 2002).

Gas Expanded Liquids as Reaction Media

The replacement of organic solvents with carbon dioxide was explored for the heterogeneously catalyzed oxidation of isopropanol to acetone with bimolecular oxygen. The use of carbon dioxide as the solvent has been shown to improve the ratio of reactants in the liquid phase and may enhance the mass transfer. Some batch experiments have been done for this reaction in a single supercritical phase at pressures above 150 bar (Gläser, Williardt et al. 2003), however addition of carbon dioxide may also be beneficial at lower pressures in the gas expanded liquid regime where the enhanced mass transfer of carbon dioxide and enhanced reactant ratios can be exploited. For other reactions where

the reactant is not a liquid or in which there is limited carbon dioxide solubility, the use of a gas expanded solvent may prove beneficial.

A continuous flow reaction system would be better to examine the optimum reaction conditions, i.e. a continuous stirred tank reactor. Here the composition in the reactor can be maintained at constant composition, removing the transient compositions present in batch reactors, and elucidate the optimum operating conditions for a gas-expanded liquid solvent. Further insight into many of the investigated reactions in the literature may be gleaned through operation in a continuous flow reactor. Some potential reactions are discussed below.

Some initial exploration of the use of CO_2-expanded liquids for homogeneously and heterogeneously catalyzed reactions has been done by Subramaniam and co-workers who have demonstrated several batch reactions in mixtures of organic solvent and carbon dioxide. The epoxidation of cyclohexenes with the homogeneous catalysts TPPFeCl and the per-fluorinated PFTPPFeCl was studied in CO_2-expanded acetonitrile (Musie, Wei et al. 2001). A maximum in conversion was observed versus composition of the liquid phase (Figure 8-2), showing the tunable nature of CO_2-expanded solvents, and gives opportunity to control the solubility of reactants and catalysts and the change the solvent properties to optimize reaction conditions. The same PFTPPFeCl catalyst was also tethered to a mesoporous material, MCM-41 and used in the heterogeneous catalyzed oxidation of cyclohexene in CO_2-expanded acetonitrile (Kerler, Robinson et al. 2004). The oxidation of cyclohexane with hydrogen peroxide as the oxidizer and pyridine as the homogeneous catalyst was performed in CO_2-expanded acetonitrile, and the oxidation of

2,6-di-tert-butylphenol was done in CO_2-expanded dichloromethane and acetonitrile (Rajagopalan, Wei et al. 2003) with Schiff base cobalt catalysts, Co(salen) and Co(salen*), with good selectivity to the desired product.

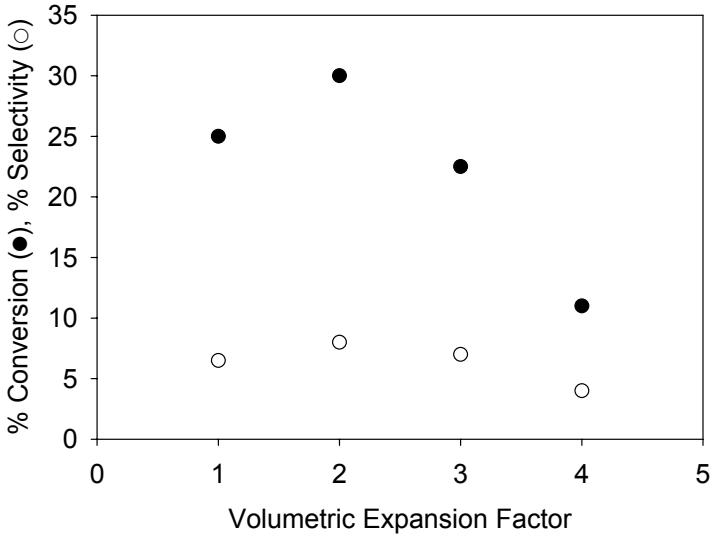

Figure 8-2. Conversion and Selectivity versus the volumetric expansion of acetonitrile for the epoxidation of cyclohexene (taken from (Musie, Wei et al. 2001))

Carbon dioxide may also offer a convenient solvent for the formation of hydrogen peroxide by reaction of hydrogen and oxygen. Baiker and coworkers have used a Pd-Pt/TS-1 catalyst to form hydrogen peroxide in situ for the epoxidation of propylene to propylene oxide in a single high pressure phase in a fixed bed reactor (Jenzer, Mallat et al. 2001) with excellent selectivity although with somewhat low yield. Beckman and coworkers have also generated hydrogen peroxide in solution for the epoxidation of cyclohexene in a carbon dioxide/water biphasic system, and found the system suitable to efficient formation of H_2O_2 (Hancu, Green et al. 2002). Other reactions that use

hydrogen peroxide as the oxidant might also benefit from the enhanced mass transfer possible with gas-expanded liquids.

The production of phenol from benzene could potentially be improved by the use of carbon dioxide as a co-solvent. Phenol production is the second largest volume chemical derived from benzene in the USA and Europe, with a worldwide production in 1996 of 4.9 million tons (Weissermel and Arpe 1997). Currently, two processes dominate the production of phenol, the Hock process and the DOW process. The Hock process uses cumene from benzene propylation that is oxidized to the hydroperoxide and disproportionated to phenol and acetone by proton-catalyzed hydroperoxide cleavage. The more recently developed DOW process oxidizes toluene to benzoic acid, which is then further oxydecarboxylated to phenol. Both of these processes are energy intensive and the Hock process suffers from the formation of large amounts of byproduct, thus there is much interest in improving this process by the single step direct oxidation of benzene.

Sen and Remias have recently proposed the hydroxylation of benzene to phenol by in situ formation of hydrogen peroxide with a palladium and vanadium or iron catalysts (Sen and Remias 2004). The have concluded that the slow step in the reaction is the formation of usable hydrogen peroxide. This may be potentially improved by the use of a gas-expanded solvent that will improve the intra-phase mass transfer.

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APPENDIX A

EQUATION OF STATE FORMULAS AND MIXING RULES

Peng-Robinson Equation of State (Peng and Robinson 1976)

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)}$$

$$a(T) = 0.457235\frac{RT_c{}^2}{P_c}\left(1+\kappa\left[1-\left(\frac{T}{T_c}\right)^{1/2}\right]\right)^2$$

$$b = 0.07780\frac{RT_c}{P_c}$$

Stryjek-Vera temperature dependency (Stryjek and Vera 1986),

$$\kappa = 0.378893 + 1.4897153\omega - 0.17131848\,\omega^2 + 0.0196554\,\omega^3 + \kappa_1\left(1+\frac{T}{T_c}\right)\left(0.7-\frac{T}{T_c}\right)$$

The compressibility of the liquid phase and the compressibility of the vapor phase are the smallest and largest roots, respectively of the cubic:

$$Z^3 + \left(\frac{bP}{RT}-1\right)Z^2 + \left(\frac{aP}{R^2T^2} - 3\left(\frac{bP}{RT}\right)^2 - 2\frac{bP}{RT}\right) - \left(\frac{aP}{R^2T^2}\frac{bP}{RT} - \left(\frac{bP}{RT}\right)^2 - \left(\frac{bP}{RT}\right)^3\right) = 0$$

Fugacity coefficient of component *i* in the mixture:

$$\ln\hat{\phi}_i = \frac{\bar{b}_i}{b}(Z-1) - \ln\frac{(V-b)Z}{V} + \frac{a/bRT}{\left(1-\sqrt{2}\right)-\left(1+\sqrt{2}\right)}\left(1+\frac{\bar{a}_i}{a}-\frac{\bar{b}_i}{b}\right)\ln\frac{V+\left(1+\sqrt{2}\right)b}{V+\left(1-\sqrt{2}\right)b}$$

Patel-Teja Equation of State (Patel and Teja 1982)

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+c(v-b)}$$

where,

$$a = \Omega_a \frac{R^2 T_c^2}{P_c}\left[1 + F\left(1 - T_R^{0.5}\right)\right]^2$$

$$b = \Omega_b \frac{RT_c}{P_c}$$

$$c = \left(1 - 3\zeta_c\right)\frac{RT_c}{P_c}$$

Ω_b is the smallest positive root of the cubic:

$$\Omega_b^3 + (2 - 3\zeta_c)\Omega_b^2 + 3\zeta_c^2\Omega_b - \zeta_c^3 = 0$$

$$\Omega_a = 3\zeta_c^2 + 3(1 - 2\zeta_c)\Omega_b + \Omega_b^2 + 1 - 3\zeta_c$$

The density of the liquid phase and the density of the vapor phase are the smallest and largest roots, respectively of the cubic:

$$v^3 + \left(c - \frac{RT}{P}\right)v^2 + \left(\frac{a}{P} - b^2 - 2bc - (b+c)\frac{RT}{P}\right)v + b^2c + \frac{bcRT - ab}{P} = 0$$

Fugacity of component *i* in the mixture:

$$RT\ln\frac{f_i}{x_i P} = -RT\ln(z-B) + RT\frac{b_i}{v-b} - \frac{\sum x_j a_{ij}}{d}\ln\frac{Q+d}{Q-d}$$

$$+\frac{a(b_i + c_i)}{2\left(Q^2 - d^2\right)} + \frac{a}{8d^3}\left\{c_i(3b+c) + b_i(3c+b)\right\}\left\{\ln\left(\frac{Q+d}{Q-d}\right) - \frac{2Qd}{Q^2 - d^2}\right\}$$

where,

$$B = \frac{bP}{RT} \qquad d = \sqrt{bc + \frac{(b+c)^2}{4}}$$

$$Q = V_m + \frac{b+c}{2}$$

Van der Waals one-fluid mixing rules

$$a = \sum\sum x_i x_j a_{ij}$$

$$a_{ij} = \left(1 - k_{ij}\right)\sqrt{a_i a_j}$$

$$b = \sum x_i b_i$$

$$c = \sum x_i c_i$$

Mathias-Klotz-Prausnitz (MKP) mixing rules (Mathias, Klotz et al. 1991)

$$a = a^{(0)} + a^{(1)}$$

$$a^{(0)} = \sum_i x_i \sum_j x_j a_{ji}^{(0)} \left(1 - k_{ji}\right)$$

$$a^{(1)} = \sum_i x_i \left(\sum_j x_j \left(a_{ji}^{(0)} l_{ji}\right)^{1/3} \right)^3$$

where,

$$a_{ji}^{(0)} = \sqrt{a_i a_j}$$

$$\bar{a}_k = \left[\frac{\partial\left(n a^{(1)}\right)}{\partial n_k} \right] = \left(\sum_j x_j \left(a_{jk}^{(0)} l_{jk}\right)^{1/3} \right)^3 + 3 \sum_i x_i \left(\sum_j x_j \left(a_{ji}^{(0)} l_{ji}\right)^{1/3} \right)^2 \left(\left(a_{ki}^{(0)} l_{ki}\right)^{1/3} - \sum_j x_j \left(a_{ji}^{(0)} l_{ji}\right)^{1/3} \right)$$

$$b = \sum x_i b_i$$

$$c = \sum x_i c_i$$

Wong-Sandler mixing rules (Wong, Orbey et al. 1992)

$$b = \frac{\sum_i \sum_j x_i x_j \left(b - \frac{a}{RT} \right)_{ij}}{1 + \frac{A^{E,\infty}}{C^* RT} - \sum_i x_i \left(\frac{a_i}{b_i RT} \right)}$$

$$\frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} - \frac{A^{E,\infty}}{RTC^*}$$

$$\left(b - \frac{a}{RT} \right)_{ij} = \frac{1}{2} \left[\left(b_i - \frac{a_i}{RT} \right) - \left(b_j - \frac{a_j}{RT} \right) \right] \left(1 - k_{ij} \right)$$

$$c = \sum x_i c_i$$

For the Peng-Robinson EoS C^* = -0.623225240140231

$$g^E(x, T, P = low) = a^E(x, T, P = low) = a^E(x, T, P = \infty)$$

k_{ij} is chosen so that the G^E calculated from the EoS matches the G^E from the activity coefficient model. Using the relation $\gamma_i^\infty = \phi_i^\infty / \phi_i$

$$\overline{a}_i = \left[\frac{\partial (na)}{\partial n_i} \right] = bRT \left(\frac{a_i}{b_i RT} - \frac{\ln \gamma_i}{C^*} \right) + a \left(\frac{\overline{b}_i}{b} - 1 \right)$$

$$\overline{b}_i = \left[\frac{\partial (nb)}{\partial n_i} \right] = \frac{2 \sum_j x_j \left(b - \frac{a}{RT} \right)_{ij} - b \left(1 + \frac{\ln \gamma_i}{C^*} - \frac{a_i}{b_i RT} \right)}{1 + \frac{A^{E,\infty}}{C^* RT} - \sum x_i \frac{a_i}{b_i RT}}$$

Huron-Vidal mixing rules (Huron and Vidal 1979)

$$\alpha = \frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} - \frac{g^{E,\infty}}{C^* RT}$$

$$b = \sum x_i b_i$$

$$c = \sum x_i c_i$$

$$\overline{\alpha}_i = \left[\frac{\partial(n\alpha)}{\partial n_i} \right] = \left(\frac{a_i}{b_i RT} - \frac{\ln \gamma_i}{C^*} \right)$$

For the Peng-Robinson EoS C^* = -0.623225240140231

Modified Huron-Vidal 1 (Michelsen 1990)

$$\alpha = \frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} + \frac{1}{q_1^{MHV1}} \left[\frac{g^{E,0}}{RT} + \sum_{i=1}^{n} x_i \ln\left(\frac{b}{b_i}\right) \right]$$

$$b = \sum x_i b_i$$

$$c = \sum x_i c_i$$

$$\overline{\alpha}_i = \left[\frac{\partial(n\alpha)}{\partial n_i} \right] = \frac{a_i}{b_i RT} + \frac{1}{q_i} \left(\ln \gamma_i + \ln\left(\frac{b}{b_i}\right) + \frac{b_i}{b} - 1 \right)$$

For the Peng-Robinson EoS q_1 = -0.52

Modified Huron-Vidal 2 (Dahl and Michelsen 1990)

$$q_1^{MHV2}\left[\alpha^{MHV2}-\sum_{i=1}^{n}x_i\alpha_i\right]+q_2^{MHV2}\left[\left(\alpha^{MHV2}\right)^2-\sum_{i=1}^{n}x_i\alpha_i^2\right]=\frac{g^{E,0}}{RT}+\sum_{i=1}^{n}x_i\ln\left(\frac{b}{b_i}\right)$$

$$b=\sum x_i b_i$$

$$c=\sum x_i c_i$$

$$\overline{\alpha}_i=\left[\frac{\partial(n\alpha)}{\partial n_i}\right]=\frac{1}{q_1+2\alpha q_2}\left[q_1\frac{a_i}{b_i RT}+q_2\left(\alpha^2-\alpha_i^2\right)+\ln\gamma_i+\ln\left(\frac{b}{b_i}\right)+\frac{b_i}{b}-1\right]$$

For the Peng-Robinson EoS q_1 = -0.41754 and q_2 = -0.0046103

Huron-Vidal-Orbey-Sandler (Orbey and Sandler 1995)

$$\alpha^{HVOS} = \frac{a}{bRT} = \sum_{i=1}^{n} x_i \frac{a_i}{b_i RT} + \frac{1}{C^*}\left[\frac{a^{E,\infty}}{RT} + \sum_{i=1}^{n} x_i \ln\left(\frac{b}{b_i}\right)\right]$$

$$b = \sum x_i b_i$$

$$c = \sum x_i c_i$$

$$g^E(x,T,P=low) = a^E(x,T,P=low) = a^E(x,T,P=\infty)$$

$$\overline{\alpha}_i = \left[\frac{\partial(n\alpha)}{\partial n_i}\right] = \frac{a_i}{b_i RT} - \frac{\ln\gamma_i}{C^*} - \frac{1}{C^*}\left(\ln\left(\frac{b}{b_i}\right) + \frac{b_i}{b} - 1\right)$$

For the Peng-Robinson EoS C^* = -0.623225240140231

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[9] Wong, D. S. H., H. Orbey, et al. (1992). "Equation of State Mixing Tule for Nonideal Mixtures Using Available Activity Coefficient Model Parameters and That Allows Extrapolation Over Large Ranges of Temperature and Pressure." *Ind. Eng. Chem. Fundam.* **31**(8): 2033-2039.

APPENDIX B

DESCRIPTION OF SAPPHIRE CELL COMPONENTS

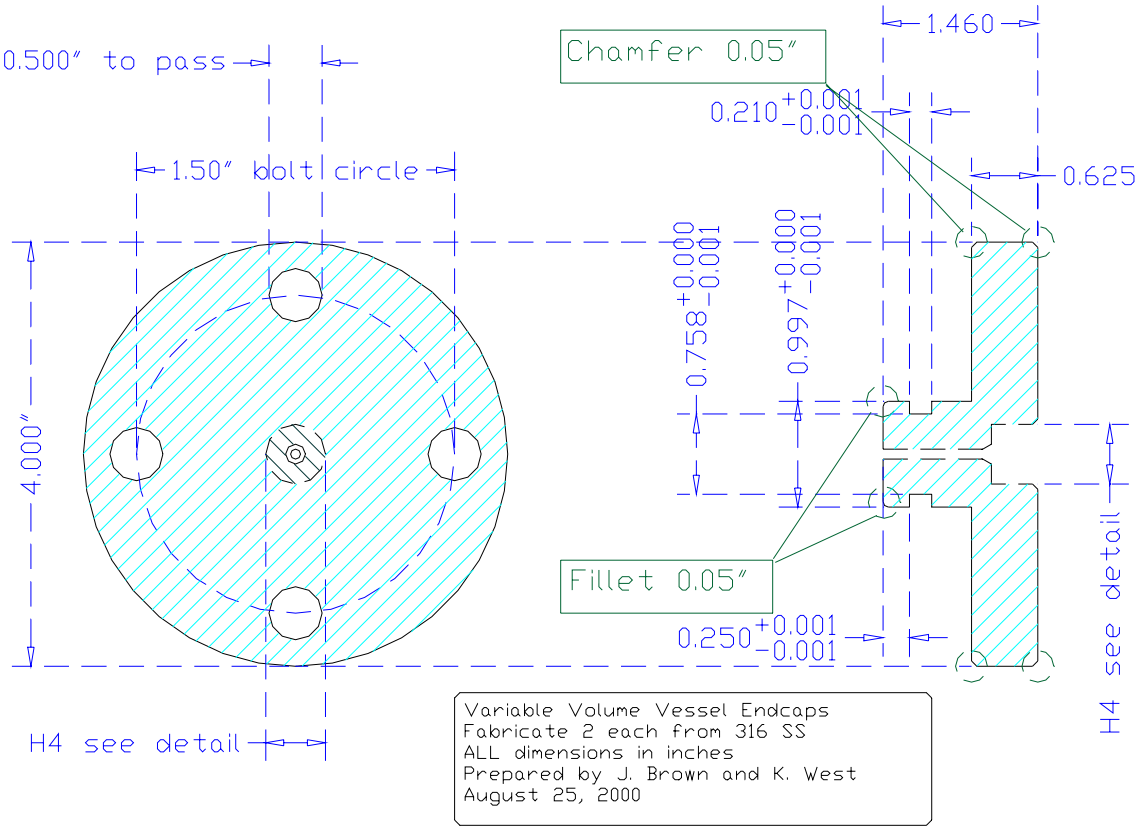

Figure B-1. Schematic diagram of the end caps used in the sapphire cell apparatus.

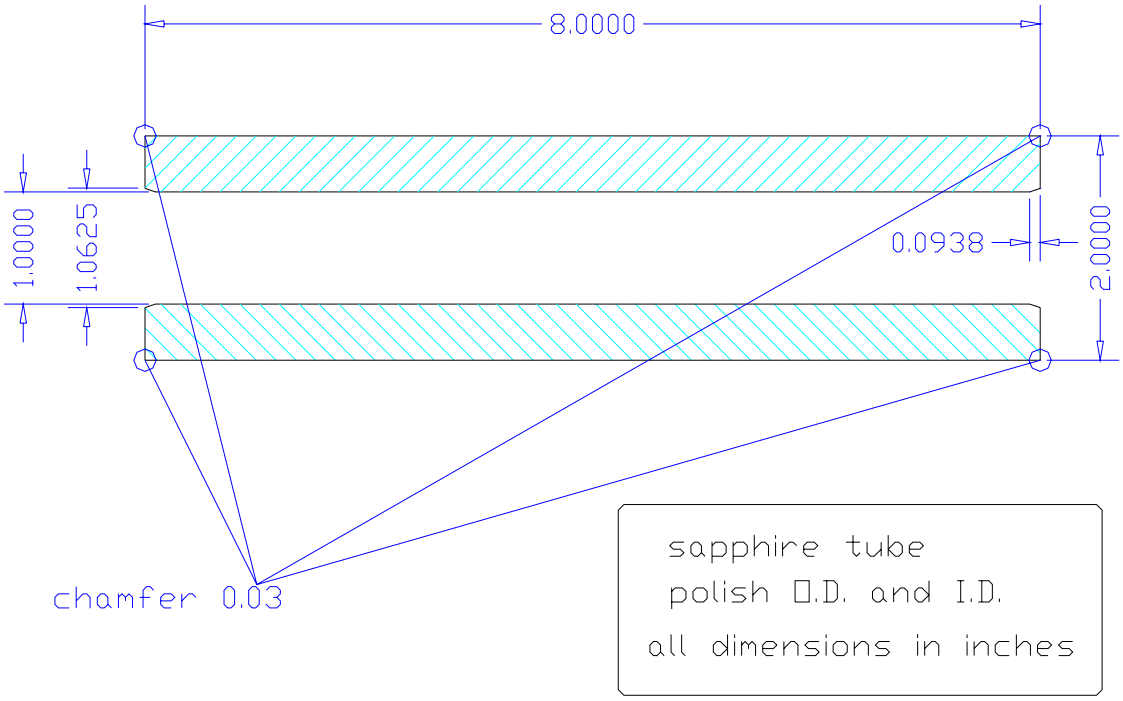

Figure B-2. Schematic diagram of the sapphire tube.

APPENDIX C

EXCESS GIBBS ENERGY AND ACTIVITY COEFFICIENT MODELS FOR MULTICOMPONENT SYSTEMS FROM ONLY PURE COMPONENT AND BINARY PARAMETERS

Wilson Model (Wilson 1964)

$$\frac{g^E}{RT} = -\sum_i^n x_i \ln\left(\sum_j^n x_j \Lambda_{ij}\right)$$

Adjustable binary parameters are Λ_{ij} ,and Λ_{ji}

Activity coefficients:

$$\ln \gamma_i = -\ln\left(\sum_j^n x_j \Lambda_{ij}\right) + 1 - \sum_k^n \frac{x_k \Lambda_{ki}}{\sum_j^n x_j \Lambda_{kj}}$$

Infinite dilution activity coefficient for a binary pair:

$$\lim_{x_1 \to 0} \gamma_1 = \gamma_1^\infty = \exp\left(-\ln \Lambda_{12} + 1 - \Lambda_{21}\right)$$

$$\lim_{x_2 \to 0} \gamma_2 = \gamma_2^\infty = \exp\left(-\ln \Lambda_{21} + 1 - \Lambda_{12}\right)$$

Non-Random Two Liquid Model (NRTL) (Renon and Prausnitz 1968)

$$\frac{g^E}{RT} = \sum_i^n x_i \frac{\sum_j^n \tau_{ji} G_{ji} x_j}{\sum_k^n G_{ki} x_k}$$

where, $\tau_{ji} = \frac{\Delta g_{ji}}{RT}$

$$G_{ji} = \exp\left(-\alpha_{ji}\tau_{ji}\right),$$

Adjustable binary parameters are Δg_{ji}, Δg_{ij}, and α_{ji} (NOTE: $\alpha_{ji} = \alpha_{ij}$)

Activity coefficients:

$$\ln \gamma_i = \frac{\sum_j^n \tau_{ji} G_{ji} x_j}{\sum_k^n G_{ki} x_k} + \sum_j^n \frac{x_j G_{ij}}{\sum_k^n G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k^n x_k \tau_{kj} G_{kj}}{\sum_k^n G_{kj} x_k} \right)$$

Infinite dilution activity coefficient for a binary pair:

$$\lim_{x_1 \to 0} \gamma_1 = \gamma_1^\infty = \exp\left(\tau_{21} + \tau_{12} G_{12}\right)$$

$$\lim_{x_2 \to 0} \gamma_2 = \gamma_2^\infty = \exp\left(\tau_{12} + \tau_{21} G_{21}\right)$$

Universal Quasi-Chemical Activity Coefficient Model (UNIQUAC) (Abrams and Prausnitz 1975)

$$\frac{g^E}{RT} = \sum_i^n x_i \ln\frac{\Phi_i}{x_i} + \frac{z}{2}\sum_i^n q_i x_i \ln\frac{\theta_i}{\Phi_i} - \sum_i^n q_i x_i \ln\sum_j^n \theta_j \tau_{ji}$$

where, $$\Phi_i = \frac{r_i x_i}{\sum_j^n r_j x_j} \qquad \theta_i = \frac{q_i x_i}{\sum_j^n q_j x_j}$$

$$\tau_{ij} = \exp\left(-\frac{u_{ij}}{RT}\right)$$

Adjustable binary parameters are u_{ij} ,and u_{ji}

r and *q* are the pure component volume and area terms, respectively

z is the coordination number set equal to 10.

Activity coefficients:

$$\ln\gamma_i = \ln\frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln\frac{\theta_i}{\Phi_i} + \ell_i - \frac{\Phi_i}{x_i}\sum_i^n x_i \ell_i$$
$$- q_i \ln\left(\sum_j^n \theta_j \tau_{ji}\right) + q_i - q_i \sum_j^n \frac{\theta_j \tau_{ij}}{\sum_k^n \theta_k \tau_{kj}}$$

where, $$\ell_i = \frac{z}{2}(r_i - q_i) - (r_i - 1)$$

Infinite dilution activity coefficient for a binary pair:

$$\lim_{x_1\to 0}\gamma_1 = \gamma_1^\infty = \exp\left(\left(\ell_1 - \frac{r_1}{r_2}\ell_2\right) - q_1 \ln\tau_{21} + q_1(1-\tau_{12})\right)$$

$$\lim_{x_2\to 0}\gamma_2 = \gamma_2^\infty = \exp\left(\left(\ell_2 - \frac{r_2}{r_1}\ell_1\right) - q_2 \ln\tau_{12} + q_2(1-\tau_{21})\right)$$

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APPENDIX D

INFINITE DILUTION ACTIVITY COEFFECIENT MODELS

Modified UNIFAC (Dortmund) (Gmehling, Li et al. 1993)

The activity coefficient is the sum of a combinatorial and a residual part:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$$

The combinatorial part:

$$\ln \gamma_i^C = 1 - V_i' + \ln V_i' - 5q_i\left(1 - \frac{V_i}{F_i} + \ln\left(\frac{V_i}{F_i}\right)\right)$$

V_i' is calculated form the van der Waals volumes R_k

$$V_i' = \frac{r_i^{3/4}}{\sum_j x_j r_j^{3/4}}$$

All other parameters are calculated in the same way as for the original UNIFAC model:

$$V_i = \frac{r_i}{\sum_j x_j r_j}$$

$$r_i = \sum \nu_k^{(i)} R_k$$

$$F_i = \frac{q_i}{\sum_j x_j q_j}$$

$$q_i = \sum \nu_k^{(i)} Q_k$$

The residual part:

$$\ln \gamma_i^R = \sum_k \nu_k^{(i)}\left(\ln \Gamma_k - \ln \Gamma_k^{(i)}\right)$$

$$\ln \Gamma_k = Q_k \left(1 - \ln\left(\sum_m \theta_m \Psi_{mk} \right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}} \right)$$

whereby the group area fraction θ_m, and group mole fraction X_m are given by the following equations,

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}$$

$$X_m = \frac{\sum_j \nu_m^{(j)} x_j}{\sum_j \sum_n \nu_n^{(j)} x_j}$$

Temperature-dependent parameters,

$$\Psi_{nm} = \exp\left(-\frac{a_{nm} + b_{nm} T + c_{nm} T^2}{T} \right)$$

References

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APPENDIX E

EXPERIMENTAL IFINITE DILUTION ACTIVITY COEFFICIENTS USED IN THE REGRESSION OF THE MOSCED PARAMETERS INCLUDING ABSOLUTE AVERAGE DEVIATION FOR BOTH THE MOSCED AND UNIFAC MODELS

Table E-1. Experimental and Predicted Infinite Dilution Activity Coefficients. References for infinite dilution activity coefficient data are in brackets [ ]. Other references are for VLE data.

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1,1,1-Trichloroethane	1,2-Dichloroethane	328.2	1.34	1.28	-4.5%	1.01	-24.6%	[1]
1,1,1-Trichloroethane	1-Octanol	298.2	1.98	1.89	-4.5%	1.37	-30.8%	[2]
1,1,1-Trichloroethane	1-Octanol	298.2	1.89	1.89	0.0%	1.37	-27.5%	[3]
1,1,1-Trichloroethane	1-Octanol	298.2	1.98	1.89	-4.5%	1.37	-30.8%	[4]
1,1,1-Trichloroethane	1-Octanol	308.2	1.76	1.83	4.0%	1.35	-23.3%	[2]
1,1,1-Trichloroethane	1-Octanol	323.2	1.63	1.76	8.0%	1.33	-18.4%	[2]
1,1,1-Trichloroethane	Anisole	293.2	1.17	1.14	-2.6%	1.18	0.9%	[5]
1,1,1-Trichloroethane	Butyl Ether	293.2	0.81	0.88	8.6%	0.84	3.7%	[5]
1,1,1-Trichloroethane	Carbon Tetrachloride	328.2	1.09	1.06	-2.8%	1.11	1.8%	[1]
1,1,1-Trichloroethane	Chloroform	328.2	1.00	0.96	-4.0%	M.P.	N.A.	[1]
1,1,1-Trichloroethane	Dichloromethane	308.2	1.18	1.17	-0.8%	1.67	41.5%	[1]
1,1,1-Trichloroethane	Dimethyl Carbonate	298.2	1.66	1.52	-8.4%	M.G.	N.A.	57
1,1,1-Trichloroethane	Dimethyl Carbonate	333.2	1.66	1.45	-12.4%	M.G.	N.A.	57
1,1,1-Trichloroethane	Methyl Isobutyl Ketone	293.2	0.87	0.93	6.9%	0.73	-16.1%	[5]
1,1,1-Trichloroethane	N-Hexadecane	298.2	1.04	1.08	4.2%	0.81	-21.8%	[6]
1,1,1-Trichloroethane	Tetraethylene Glycol DME	303.2	0.72	0.78	8.2%	0.69	-4.3%	[7]
1,1,1-Trichloroethane	Tetraethylene Glycol DME	323.2	0.74	0.80	7.7%	0.76	2.3%	[7]
1,1,1-Trichloroethane	Tetraethylene Glycol DME	343.5	0.79	0.81	3.2%	0.80	1.9%	[7]
1,1,1-Trichloroethane	Tributyl Phosphate	298.2	0.50	0.48	-4.0%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Tributyl Phosphate	303.2	0.50	0.48	-4.0%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Tributyl Phosphate	308.2	0.51	0.49	-3.9%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Tributyl Phosphate	313.2	0.51	0.50	-2.0%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Tributyl Phosphate	318.2	0.51	0.50	-2.0%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Tributyl Phosphate	323.2	0.51	0.51	0.0%	M.G.	N.A.	[8]
1,1,1-Trichloroethane	Trichloroethylene	328.2	1.02	0.99	-2.9%	0.99	-2.9%	[9]
1,1-Dichloroethane	1,1,1-Trichloroethane	328.2	1.06	1.28	20.8%	1.11	4.7%	[1]
1,1-Dichloroethane	1,2-Dichloroethane	328.2	1.14	1.01	-11.4%	1.09	-4.4%	[1]
1,1-Dichloroethane	1-Octanol	298.2	2.01	2.04	1.5%	1.61	-19.9%	[2]
1,1-Dichloroethane	1-Octanol	298.2	2.01	2.04	1.5%	1.61	-19.9%	[4]
1,1-Dichloroethane	1-Octanol	308.2	2.01	1.96	-2.5%	1.58	-21.4%	[2]
1,1-Dichloroethane	1-Octanol	323.2	1.90	1.85	-2.6%	1.55	-18.4%	[2]
1,1-Dichloroethane	Carbon Tetrachloride	328.2	1.40	1.66	18.6%	1.23	-12.1%	[1]
1,1-Dichloroethane	Chloroform	328.2	0.98	1.01	3.1%	0.98	0.0%	[1]
1,1-Dichloroethane	Dichloromethane	308.2	1.02	0.98	-3.9%	1.06	3.9%	[1]
1,1-Dichloroethane	Trichloroethylene	328.2	1.26	1.33	5.6%	1.00	-20.6%	[9]
1,2-Dichloroethane	1,1,1-Trichloroethane	328.2	1.23	1.30	5.7%	1.03	-16.3%	[1]
1,2-Dichloroethane	1-Butanol	293.2	2.92	3.31	13.4%	2.45	-16.1%	[10]
1,2-Dichloroethane	1-Octanol	298.2	2.68	2.33	-13.1%	2.55	-4.9%	[2]
1,2-Dichloroethane	1-Octanol	298.2	2.41	2.33	-3.3%	2.55	5.8%	[3]
1,2-Dichloroethane	1-Octanol	298.2	2.68	2.33	-13.1%	2.55	-4.9%	[4]
1,2-Dichloroethane	1-Octanol	308.2	2.55	2.22	-12.9%	2.42	-5.1%	[2]
1,2-Dichloroethane	1-Octanol	323.2	2.31	2.07	-10.4%	2.25	-2.6%	[2]
1,2-Dichloroethane	Acetone	329.4	0.98	0.91	-7.1%	0.29	-70.4%	[11]
1,2-Dichloroethane	Acetonitrile	333.2	1.52	1.64	8.2%	0.51	-66.4%	123
1,2-Dichloroethane	Anisole	293.2	0.94	0.88	-6.4%	0.18	-80.9%	[5]
1,2-Dichloroethane	Benzene	298.2	1.04	1.09	4.8%	0.63	-39.4%	121
1,2-Dichloroethane	Benzene	353.3	1.03	1.07	3.9%	0.65	-36.9%	[11]
1,2-Dichloroethane	Benzyl Acetate	298.2	0.71	0.75	5.6%	0.38	-46.5%	[10]
1,2-Dichloroethane	Butyl Ether	293.2	1.17	1.30	11.1%	0.57	-51.3%	[5]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1,2-Dichloroethane	Carbon Tetrachloride	313.2	1.73	1.80	3.9%	1.74	0.4%	408
1,2-Dichloroethane	Carbon Tetrachloride	328.2	1.65	1.72	4.2%	1.64	-0.6%	[1]
1,2-Dichloroethane	Chloroform	328.2	1.05	1.02	-2.9%	0.82	-21.9%	[1]
1,2-Dichloroethane	Cyclohexane	298.2	3.32	3.59	8.1%	4.44	33.7%	120
1,2-Dichloroethane	Cyclohexane	334.2	2.52	2.79	10.7%	3.07	21.8%	[12]
1,2-Dichloroethane	Cyclohexane	340.4	2.44	2.69	10.2%	2.91	19.3%	[12]
1,2-Dichloroethane	Cyclohexane	345.7	2.36	2.62	11.0%	2.78	17.8%	[12]
1,2-Dichloroethane	Cyclohexane	351.2	2.29	2.54	10.9%	2.65	15.7%	[12]
1,2-Dichloroethane	Dichloromethane	308.2	0.99	0.98	-1.0%	1.11	12.1%	[1]
1,2-Dichloroethane	Ethyl Acetate	311.7	0.81	0.83	2.5%	0.44	-45.7%	[12]
1,2-Dichloroethane	Ethyl Acetate	330.5	0.83	0.86	3.6%	0.47	-43.4%	[12]
1,2-Dichloroethane	Ethyl Acetate	347.8	0.85	0.88	3.5%	0.49	-42.4%	[12]
1,2-Dichloroethane	Methanol	323.2	4.95	6.18	24.7%	2.67	-46.1%	314
1,2-Dichloroethane	Methyl Ethyl Ketone	314.7	0.77	0.74	-3.9%	0.31	-59.7%	[12]
1,2-Dichloroethane	Methyl Ethyl Ketone	333.2	0.74	0.77	4.2%	0.34	-54.0%	122
1,2-Dichloroethane	Methyl Ethyl Ketone	333.3	0.79	0.77	-2.5%	0.34	-57.0%	[12]
1,2-Dichloroethane	Methyl Ethyl Ketone	350.3	0.82	0.80	-2.4%	0.36	-56.1%	[12]
1,2-Dichloroethane	Methyl Isobutyl Ketone	293.2	0.69	0.77	11.6%	0.35	-49.3%	[5]
1,2-Dichloroethane	N,N-Dibutylformamide	302.8	0.51	0.44	-13.2%	0.13	-74.4%	[13]
1,2-Dichloroethane	N,N-Dibutylformamide	318.3	0.51	0.48	-6.1%	0.15	-70.6%	[13]
1,2-Dichloroethane	N,N-Dibutylformamide	332.4	0.52	0.50	-4.6%	0.17	-67.6%	[13]
1,2-Dichloroethane	N,N-Dimethylacetamide	303.6	0.54	0.48	-11.8%	0.07	-87.1%	[13]
1,2-Dichloroethane	N,N-Dimethylacetamide	317.6	0.63	0.52	-18.0%	0.08	-87.4%	[13]
1,2-Dichloroethane	N,N-Dimethylacetamide	333.4	0.75	0.56	-25.0%	0.10	-86.6%	[13]
1,2-Dichloroethane	N-Heptane	293.2	3.30	3.67	11.2%	4.27	29.4%	[10]
1,2-Dichloroethane	N-Hexadecane	298.2	2.34	2.40	2.5%	3.14	34.2%	118
1,2-Dichloroethane	N-Hexadecane	298.2	2.03	2.40	18.1%	3.14	54.5%	[6]
1,2-Dichloroethane	N-Hexane	298.0	3.17	3.76	18.6%	4.35	37.2%	[12]
1,2-Dichloroethane	N-Hexane	298.2	3.61	3.75	4.0%	4.35	20.6%	119
1,2-Dichloroethane	N-Hexane	316.0	2.73	3.26	19.4%	3.89	42.5%	[12]
1,2-Dichloroethane	N-Hexane	333.2	2.45	2.91	18.8%	3.49	42.4%	[12]
1,2-Dichloroethane	N-Hexane	339.4	2.32	2.80	20.7%	3.35	44.4%	[12]
1,2-Dichloroethane	Nitrobenzene	293.2	1.09	0.96	-11.9%	M.P.	N.A.	[10]
1,2-Dichloroethane	N-Methylacetamide	303.4	1.60	1.77	10.6%	M.P.	N.A.	[13]
1,2-Dichloroethane	N-Methylacetamide	318.4	1.62	1.75	8.0%	M.P.	N.A.	[13]
1,2-Dichloroethane	N-Methylacetamide	333.2	1.64	1.71	4.4%	M.P.	N.A.	[13]
1,2-Dichloroethane	N-Octane	293.2	2.90	3.47	19.7%	4.10	41.4%	[10]
1,2-Dichloroethane	Phenol	323.2	1.72	2.40	39.5%	M.P.	N.A.	[10]
1,2-Dichloroethane	Phenol	328.2	2.41	2.38	-1.2%	M.P.	N.A.	[14]
1,2-Dichloroethane	Phenol	343.2	2.14	2.31	7.9%	M.P.	N.A.	[14]
1,2-Dichloroethane	Phenol	358.2	2.03	2.23	9.9%	M.P.	N.A.	[14]
1,2-Dichloroethane	Phenol	373.2	2.03	2.15	5.9%	M.P.	N.A.	[14]
1,2-Dichloroethane	Quinoline	298.2	0.92	0.92	0.0%	M.G.	N.A.	[10]
1,2-Dichloroethane	Sulfolane	303.1	1.13	1.22	7.8%	M.G.	N.A.	[13]
1,2-Dichloroethane	Sulfolane	317.9	1.17	1.21	3.7%	M.G.	N.A.	[13]
1,2-Dichloroethane	Sulfolane	333.6	1.21	1.19	-1.5%	M.G.	N.A.	[13]
1,2-Dichloroethane	Tetraethylene Glycol DME	303.2	0.32	0.40	26.6%	0.04	-87.3%	[7]
1,2-Dichloroethane	Tetraethylene Glycol DME	323.2	0.38	0.44	15.8%	0.08	-78.9%	[7]
1,2-Dichloroethane	Tetraethylene Glycol DME	343.2	0.44	0.47	8.0%	0.19	-56.3%	[7]
1,2-Dichloroethane	Tetrahydrofuran	303.2	0.45	0.64	42.2%	0.24	-46.7%	[15]
1,2-Dichloroethane	Tetrahydrofuran	323.2	0.56	0.69	23.2%	0.26	-53.6%	[15]
1,2-Dichloroethane	Tetrahydrofuran	343.2	0.60	0.73	21.7%	0.28	-53.3%	[15]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1,2-Dichloroethane	Toluene	342.7	0.95	1.13	18.9%	0.60	-36.8%	[12]
1,2-Dichloroethane	Toluene	380.9	0.97	1.11	14.4%	0.63	-35.1%	[12]
1,2-Dichloroethane	Tributyl Phosphate	298.2	0.29	0.30	3.4%	M.G.	N.A.	[8]
1,2-Dichloroethane	Tributyl Phosphate	303.2	0.29	0.31	6.9%	M.G.	N.A.	[8]
1,2-Dichloroethane	Tributyl Phosphate	308.2	0.29	0.32	10.3%	M.G.	N.A.	[8]
1,2-Dichloroethane	Tributyl Phosphate	313.2	0.29	0.33	13.8%	M.G.	N.A.	[8]
1,2-Dichloroethane	Tributyl Phosphate	318.2	0.30	0.33	10.0%	M.G.	N.A.	[8]
1,2-Dichloroethane	Tributyl Phosphate	323.2	0.30	0.34	13.3%	M.G.	N.A.	[8]
1,2-Dichloroethane	Trichloroethylene	328.2	1.42	1.36	-4.2%	0.86	-39.4%	[9]
1,2-Dichloroethane	Triethylamine	323.5	1.44	1.47	2.1%	0.56	-61.1%	[12]
1,2-Dichloroethane	Triethylamine	348.7	1.40	1.42	1.4%	0.46	-67.1%	[12]
1,2-Dichloroethane	Triethylamine	359.3	1.35	1.40	3.7%	0.42	-68.9%	[12]
1,4-Dioxane	1-Butanol	298.2	2.42	2.35	-2.9%	2.69	11.2%	[16]
1,4-Dioxane	1-Octanol	298.2	2.18	2.31	6.0%	2.12	-2.8%	[3]
1,4-Dioxane	1-Octanol	298.2	2.08	2.31	11.1%	2.12	1.9%	[16]
1,4-Dioxane	2,2,4-Trimethylpentane	298.2	3.55	5.44	53.2%	4.05	14.1%	[16]
1,4-Dioxane	2,6-Dimethylpyridine	298.2	1.02	1.24	21.6%	1.44	41.2%	[16]
1,4-Dioxane	2-Methyl-2-Propanol	298.2	1.64	2.23	36.0%	3.06	86.6%	[16]
1,4-Dioxane	Acetic Acid	298.2	0.44	0.70	59.1%	0.45	2.3%	[16]
1,4-Dioxane	Acetone	298.2	1.29	1.50	16.3%	1.34	3.9%	[16]
1,4-Dioxane	Acetone	298.3	1.35	1.50	11.1%	1.34	-0.7%	[17]
1,4-Dioxane	Acetone	308.2	1.39	1.48	6.5%	1.33	-4.3%	[17]
1,4-Dioxane	Acetone	318.4	1.36	1.46	7.4%	1.32	-2.9%	[17]
1,4-Dioxane	Acetone	328.4	1.37	1.44	5.1%	1.31	-4.4%	[17]
1,4-Dioxane	Acetonitrile	298.2	1.37	1.73	26.3%	1.28	-6.6%	[16]
1,4-Dioxane	Acetonitrile	313.2	1.45	1.66	14.3%	1.29	-11.2%	226
1,4-Dioxane	Acetophenone	298.2	0.86	0.87	1.2%	0.92	7.0%	[16]
1,4-Dioxane	Aniline	298.2	0.38	0.80	110.5%	M.P.	N.A.	[16]
1,4-Dioxane	Anisole	298.2	0.87	0.88	1.1%	0.91	4.6%	[16]
1,4-Dioxane	Benzene	298.2	0.97	1.03	6.2%	1.03	6.2%	[16]
1,4-Dioxane	Benzonitrile	298.2	0.82	1.10	34.1%	M.G.	N.A.	[16]
1,4-Dioxane	Benzyl Alcohol	298.2	0.47	0.60	27.7%	1.36	189.4%	[16]
1,4-Dioxane	Bromobenzene	298.2	0.99	1.14	15.2%	0.96	-3.0%	[16]
1,4-Dioxane	Bromoethane	298.2	1.32	1.15	-12.9%	1.62	22.7%	[16]
1,4-Dioxane	Butyl Ether	298.2	2.07	2.25	8.7%	1.94	-6.3%	[16]
1,4-Dioxane	Butyronitrile	298.2	1.14	1.20	5.3%	0.26	-77.2%	[16]
1,4-Dioxane	Carbon Disulfide	298.2	3.64	3.01	-17.3%	3.82	4.9%	[16]
1,4-Dioxane	Carbon Disulfide	298.3	3.77	3.01	-20.2%	3.82	1.3%	[17]
1,4-Dioxane	Carbon Disulfide	308.4	3.56	2.85	-19.9%	3.57	0.3%	[17]
1,4-Dioxane	Carbon Disulfide	318.7	3.34	2.70	-19.2%	3.34	0.0%	[17]
1,4-Dioxane	Carbon Tetrachloride	298.2	1.29	1.52	17.7%	1.41	9.2%	32
1,4-Dioxane	Carbon Tetrachloride	298.2	1.25	1.52	21.6%	1.41	12.8%	[16]
1,4-Dioxane	Carbon Tetrachloride	303.2	1.32	1.51	14.4%	1.42	7.6%	32
1,4-Dioxane	Carbon Tetrachloride	308.2	1.33	1.50	12.5%	1.42	6.5%	32
1,4-Dioxane	Carbon Tetrachloride	313.2	1.34	1.49	11.1%	1.43	6.7%	32
1,4-Dioxane	Carbon Tetrachloride	313.2	1.32	1.49	12.9%	1.43	8.3%	[15]
1,4-Dioxane	Carbon Tetrachloride	337.7	1.34	1.44	7.5%	1.44	7.5%	[15]
1,4-Dioxane	Chlorobenzene	298.2	0.94	1.16	23.4%	0.98	4.3%	[16]
1,4-Dioxane	Chloroform	298.2	0.22	0.21	-4.5%	0.08	-63.6%	[16]
1,4-Dioxane	Chloroform	303.2	0.19	0.22	18.6%	0.09	-51.5%	210
1,4-Dioxane	Chloroform	323.2	0.27	0.28	4.8%	0.11	-58.8%	210
1,4-Dioxane	Cyclohexane	298.2	4.17	4.58	9.8%	5.93	42.2%	[16]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1,4-Dioxane	Cyclohexanone	298.2	1.04	1.04	0.0%	1.25	20.2%	[16]
1,4-Dioxane	Dichloromethane	298.2	0.42	0.39	-7.1%	0.37	-11.9%	[16]
1,4-Dioxane	Dichloromethane	303.2	0.41	0.40	-1.4%	0.38	-6.3%	199
1,4-Dioxane	Diethyl Ether	298.2	1.96	2.22	13.3%	1.96	0.0%	[16]
1,4-Dioxane	Diisopropyl Ether	298.2	2.15	2.39	11.2%	2.30	7.0%	[16]
1,4-Dioxane	Dimethyl Sulfoxide	298.2	1.63	2.04	25.2%	M.P.	N.A.	[16]
1,4-Dioxane	Ethanol	298.2	3.10	2.60	-16.1%	3.34	7.7%	[16]
1,4-Dioxane	Ethanol	323.2	2.84	2.42	-14.8%	2.73	-3.9%	339
1,4-Dioxane	Ethanol	323.2	2.89	2.42	-16.3%	2.73	-5.6%	339
1,4-Dioxane	Ethyl Acetate	298.2	1.08	1.25	15.7%	1.07	-0.9%	[16]
1,4-Dioxane	Ethyl Acetate	328.4	1.10	1.22	10.9%	1.10	0.0%	[17]
1,4-Dioxane	Isopropanol	298.2	3.01	2.86	-5.0%	2.90	-3.7%	[16]
1,4-Dioxane	Isopropanol	323.2	2.32	2.59	11.8%	2.33	0.6%	330
1,4-Dioxane	Isopropanol	333.2	2.19	2.51	14.4%	2.16	-1.6%	330
1,4-Dioxane	Isopropanol	343.2	2.46	2.42	-1.5%	2.01	-18.2%	330
1,4-Dioxane	Isopropanol	353.2	2.30	2.35	2.3%	1.87	-18.6%	330
1,4-Dioxane	Methanol	298.2	3.39	2.35	-30.7%	2.85	-15.9%	[16]
1,4-Dioxane	Methanol	308.7	3.23	2.29	-29.1%	2.72	-15.8%	[17]
1,4-Dioxane	Methanol	318.5	3.12	2.23	-28.5%	2.59	-17.0%	[17]
1,4-Dioxane	Methanol	328.5	2.98	2.17	-27.2%	2.46	-17.4%	[17]
1,4-Dioxane	Methanol	337.0	2.88	2.12	-26.4%	2.35	-18.4%	[17]
1,4-Dioxane	Methyl Ethyl Ketone	298.2	1.17	1.18	0.9%	1.19	1.7%	[18]
1,4-Dioxane	N,N-Dibutylformamide	302.8	1.20	0.96	-19.8%	1.31	9.4%	[13]
1,4-Dioxane	N,N-Dibutylformamide	318.3	1.08	0.95	-12.1%	1.26	16.6%	[13]
1,4-Dioxane	N,N-Dibutylformamide	332.4	1.06	0.94	-11.2%	1.21	14.3%	[13]
1,4-Dioxane	N,N-Dimethylacetamide	303.3	1.33	1.18	-11.2%	M.P.	N.A.	[13]
1,4-Dioxane	N,N-Dimethylacetamide	317.6	1.29	1.17	-9.4%	M.P.	N.A.	[13]
1,4-Dioxane	N,N-Dimethylacetamide	333.6	1.26	1.15	-8.4%	M.P.	N.A.	[13]
1,4-Dioxane	N,N-Dimethylformamide	298.2	1.23	1.45	17.9%	1.30	5.7%	[16]
1,4-Dioxane	N-Decane	298.2	3.15	4.04	28.3%	3.64	15.6%	[16]
1,4-Dioxane	N-Heptane	298.2	4.41	4.74	7.5%	4.33	-1.8%	33
1,4-Dioxane	N-Heptane	298.2	3.81	4.74	24.4%	4.33	13.6%	[16]
1,4-Dioxane	N-Heptane	303.2	4.17	4.52	8.4%	4.12	-1.2%	33
1,4-Dioxane	N-Heptane	308.2	3.88	4.32	11.3%	3.93	1.3%	33
1,4-Dioxane	N-Heptane	313.2	3.69	4.13	11.8%	3.75	1.5%	33
1,4-Dioxane	N-Heptane	313.4	3.59	4.13	15.0%	3.75	4.5%	[19]
1,4-Dioxane	N-Heptane	333.2	3.21	3.54	10.3%	3.17	-1.2%	[19]
1,4-Dioxane	N-Heptane	353.2	2.76	3.10	12.2%	2.73	-1.2%	33
1,4-Dioxane	N-Heptane	353.2	2.63	3.10	17.9%	2.73	3.8%	[19]
1,4-Dioxane	N-Hexadecane	298.2	2.78	3.19	14.7%	2.90	4.3%	[6]
1,4-Dioxane	N-Hexadecane	298.2	2.42	3.19	31.8%	2.90	19.8%	[16]
1,4-Dioxane	N-Hexane	298.2	4.03	5.09	26.3%	4.70	16.6%	[16]
1,4-Dioxane	N-Hexane	353.2	3.09	3.31	7.1%	2.96	-4.2%	339
1,4-Dioxane	Nitrobenzene	298.2	0.82	0.90	9.8%	M.P.	N.A.	[16]
1,4-Dioxane	N-Methylacetamide	303.0	2.49	2.00	-19.5%	M.P.	N.A.	[13]
1,4-Dioxane	N-Methylacetamide	318.4	2.42	1.96	-19.1%	M.P.	N.A.	[13]
1,4-Dioxane	N-Methylacetamide	333.3	2.30	1.91	-17.0%	M.P.	N.A.	[13]
1,4-Dioxane	N-Octane	353.2	2.58	2.93	13.5%	2.56	-0.8%	198
1,4-Dioxane	N-Pentane	298.2	4.76	5.67	19.1%	5.23	9.9%	[16]
1,4-Dioxane	P-Xylene	298.2	1.25	1.40	12.0%	1.26	0.8%	[16]
1,4-Dioxane	Pyridine	298.2	0.96	1.16	20.8%	1.17	21.9%	[16]
1,4-Dioxane	Sulfolane	317.9	1.48	1.61	8.9%	M.G.	N.A.	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1,4-Dioxane	Sulfolane	332.7	1.28	1.55	21.5%	M.G.	N.A.	[13]
1,4-Dioxane	Tetraethylene Glycol DME	303.2	0.74	0.80	7.8%	0.78	5.1%	[7]
1,4-Dioxane	Tetraethylene Glycol DME	323.2	0.75	0.79	4.8%	0.74	-1.9%	[7]
1,4-Dioxane	Tetraethylene Glycol DME	343.2	0.77	0.79	3.3%	0.71	-7.2%	[7]
1,4-Dioxane	Tetrahydrofuran	298.2	1.13	1.22	8.0%	1.25	10.6%	[16]
1,4-Dioxane	Toluene	298.2	1.15	1.17	1.7%	1.16	0.9%	[16]
1,4-Dioxane	Tributyl Phosphate	318.2	0.86	0.75	-12.8%	M.G.	N.A.	[20]
1,4-Dioxane	Tributyl Phosphate	333.2	0.78	0.73	-6.4%	M.G.	N.A.	[20]
1,4-Dioxane	Tributyl Phosphate	363.2	0.55	0.72	30.9%	M.G.	N.A.	[20]
1,4-Dioxane	Tributyl Phosphate	373.2	0.56	0.71	26.8%	M.G.	N.A.	[20]
1,4-Dioxane	Triethylamine	298.2	2.50	3.45	38.0%	M.P.	N.A.	[16]
1-Butanol	1-Octanol	298.2	1.11	1.06	-4.5%	1.06	-4.5%	[3]
1-Butanol	1-Propanol	313.2	1.04	0.97	-7.0%	1.01	-3.2%	3
1-Butanol	1-Propanol	333.2	1.02	0.97	-4.9%	1.01	-1.0%	[21]
1-Butanol	1-Propanol	353.2	1.02	0.97	-4.9%	1.01	-1.0%	[21]
1-Butanol	2,6-Dimethylpyridine	313.2	0.70	0.77	9.5%	1.34	90.6%	166
1-Butanol	2-Methyl-1-Propanol	313.2	1.04	1.01	-2.8%	1.00	-3.8%	14
1-Butanol	2-Methyl-2-Propanol	313.2	0.80	0.99	23.1%	1.23	52.9%	8
1-Butanol	Acetonitrile	333.2	3.28	3.80	15.8%	2.94	-10.4%	130
1-Butanol	Alpha-Pinene	353.2	7.28	8.09	11.1%	6.68	-8.2%	[22]
1-Butanol	Alpha-Pinene	373.2	6.29	6.15	-2.2%	4.82	-23.4%	[22]
1-Butanol	Anisole	353.2	4.20	4.15	-1.3%	2.43	-42.2%	50
1-Butanol	Butyronitrile	278.2	4.55	4.36	-4.1%	1.76	-61.3%	27
1-Butanol	Butyronitrile	288.2	4.33	3.97	-8.2%	1.75	-59.5%	27
1-Butanol	Butyronitrile	293.2	3.98	3.80	-4.6%	1.73	-56.6%	27
1-Butanol	Butyronitrile	298.2	3.64	3.65	0.2%	1.71	-53.1%	27
1-Butanol	Butyronitrile	303.2	3.47	3.51	1.3%	1.68	-51.5%	27
1-Butanol	Butyronitrile	308.2	3.34	3.38	1.2%	1.64	-50.9%	27
1-Butanol	Butyronitrile	313.2	3.14	3.26	3.7%	1.60	-49.1%	27
1-Butanol	Butyronitrile	323.2	2.84	3.05	7.6%	1.52	-46.4%	27
1-Butanol	Cyclohexane	312.9	28.13	24.49	-12.9%	32.38	15.1%	[17]
1-Butanol	Cyclohexane	318.2	20.06	21.46	7.0%	27.69	38.1%	159
1-Butanol	Cyclohexane	322.9	21.46	19.21	-10.5%	24.20	12.8%	[17]
1-Butanol	Cyclohexane	333.0	16.47	15.42	-6.4%	18.35	11.4%	[17]
1-Butanol	Cyclohexane	343.0	13.31	12.68	-4.7%	14.20	6.7%	[17]
1-Butanol	Cyclohexane	352.9	11.05	10.65	-3.6%	11.21	1.4%	[17]
1-Butanol	Di-N-Propyl Ether	278.2	5.61	7.51	33.9%	5.06	-9.8%	72
1-Butanol	Di-N-Propyl Ether	288.2	5.30	6.34	19.7%	4.65	-12.2%	72
1-Butanol	Di-N-Propyl Ether	293.2	5.14	5.87	14.2%	4.46	-13.2%	72
1-Butanol	Di-N-Propyl Ether	298.2	4.97	5.46	9.8%	4.29	-13.8%	72
1-Butanol	Di-N-Propyl Ether	303.2	4.88	5.10	4.5%	4.13	-15.4%	72
1-Butanol	Di-N-Propyl Ether	308.2	4.64	4.78	3.1%	3.98	-14.2%	72
1-Butanol	Di-N-Propyl Ether	313.2	4.48	4.49	0.1%	3.84	-14.4%	72
1-Butanol	Di-N-Propyl Ether	323.2	4.22	4.01	-5.0%	3.59	-14.9%	72
1-Butanol	Ethanol	313.2	1.10	1.06	-3.5%	1.07	-2.6%	4
1-Butanol	Isopropanol	313.2	0.98	1.03	4.8%	1.02	3.8%	13
1-Butanol	Methanol	313.2	1.30	1.19	-8.6%	1.16	-10.9%	5
1-Butanol	Methyl Ethyl Ketone	278.2	2.82	2.55	-9.5%	2.69	-4.5%	79
1-Butanol	Methyl Ethyl Ketone	288.2	2.54	2.40	-5.4%	2.44	-3.8%	79
1-Butanol	Methyl Ethyl Ketone	293.2	2.43	2.34	-3.6%	2.34	-3.6%	79
1-Butanol	Methyl Ethyl Ketone	298.2	2.29	2.28	-0.4%	2.24	-2.2%	79
1-Butanol	Methyl Ethyl Ketone	303.2	2.23	2.23	0.1%	2.16	-3.0%	79

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Butanol	Methyl Ethyl Ketone	308.2	2.19	2.17	-1.0%	2.07	-5.6%	79
1-Butanol	Methyl Ethyl Ketone	313.2	2.10	2.13	1.4%	2.00	-4.7%	79
1-Butanol	Methyl Ethyl Ketone	323.2	1.98	2.04	2.8%	1.87	-5.7%	79
1-Butanol	N,N-Dibutylformamide	332.5	0.72	0.67	-6.7%	0.95	32.3%	[13]
1-Butanol	N,N-Dimethylacetamide	333.4	0.79	0.63	-19.8%	0.57	-27.5%	[13]
1-Butanol	N-Decane	293.2	39.60	34.36	-13.2%	34.61	-12.6%	[23]
1-Butanol	N-Dodecane	293.2	38.70	33.40	-13.7%	31.65	-18.2%	[23]
1-Butanol	N-Heptane	333.2	14.12	12.98	-8.1%	15.82	12.0%	144
1-Butanol	N-Heptane	353.2	9.30	9.00	-3.2%	10.60	14.0%	[21]
1-Butanol	N-Heptane	363.2	8.70	7.69	-11.6%	8.82	1.4%	144
1-Butanol	N-Heptane	373.2	5.62	6.67	18.7%	7.40	31.7%	[21]
1-Butanol	N-Hexadecane	293.2	34.50	30.89	-10.5%	27.42	-20.5%	[23]
1-Butanol	N-Hexadecane	298.2	27.74	26.33	-5.1%	23.95	-13.7%	[6]
1-Butanol	N-Hexane	301.0	33.00	28.97	-12.2%	36.77	11.4%	[12]
1-Butanol	N-Hexane	315.3	22.50	19.75	-12.2%	25.78	14.6%	[12]
1-Butanol	N-Hexane	331.8	15.10	13.61	-9.9%	17.78	17.7%	[12]
1-Butanol	N-Hexane	333.2	14.31	13.23	-7.5%	17.26	20.6%	143
1-Butanol	N-Hexane	340.3	12.20	11.52	-5.6%	14.90	22.1%	[12]
1-Butanol	N-Methylacetamide	303.1	1.27	0.99	-22.0%	1.03	-18.9%	[13]
1-Butanol	N-Methylacetamide	318.4	1.10	0.98	-10.6%	1.00	-8.8%	[13]
1-Butanol	N-Methylacetamide	333.2	0.97	0.97	-0.1%	1.00	3.0%	[13]
1-Butanol	N-Octane	293.2	42.20	35.56	-15.7%	38.70	-8.3%	[23]
1-Butanol	N-Tetradecane	293.2	35.70	32.08	-10.1%	29.33	-17.8%	[23]
1-Butanol	P-Xylene	313.2	9.48	10.67	12.6%	8.08	-14.8%	62
1-Butanol	Pyridine	313.2	1.07	0.96	-10.4%	0.64	-40.3%	182
1-Butanol	Sulfolane	303.1	5.35	4.73	-11.7%	M.G.	N.A.	[13]
1-Butanol	Sulfolane	317.9	4.49	4.22	-6.1%	M.G.	N.A.	[13]
1-Butanol	Sulfolane	333.6	3.70	3.80	2.7%	M.G.	N.A.	[13]
1-Butanol	Toluene	353.2	4.70	5.37	14.3%	4.34	-7.7%	[24]
1-Butanol	Toluene	363.2	4.10	4.80	17.1%	3.86	-5.9%	[24]
1-Butanol	Toluene	373.2	3.62	4.34	19.9%	3.50	-3.3%	[24]
1-Butanol	Toluene	383.2	3.18	3.96	24.5%	3.23	1.6%	[24]
1-Chlorobutane	1-Octanol	298.2	2.24	2.14	-4.5%	1.98	-11.6%	[3]
1-Chlorobutane	Acetonitrile	323.2	4.71	3.75	-20.4%	3.79	-19.5%	[25]
1-Chlorobutane	Acetonitrile	348.2	3.98	3.12	-21.6%	3.28	-17.6%	[25]
1-Chlorobutane	Cyclohexane	315.1	1.56	1.65	5.8%	1.40	-10.3%	[12]
1-Chlorobutane	Cyclohexane	325.8	1.52	1.60	5.3%	1.36	-10.5%	[12]
1-Chlorobutane	Cyclohexane	340.7	1.46	1.55	6.2%	1.31	-10.3%	[12]
1-Chlorobutane	Cyclohexane	350.8	1.43	1.52	6.3%	1.29	-9.8%	[12]
1-Chlorobutane	Ethyl Acetate	323.2	1.25	1.18	-5.6%	1.17	-6.4%	[25]
1-Chlorobutane	Ethyl Acetate	348.2	1.23	1.16	-5.7%	1.15	-6.5%	[26]
1-Chlorobutane	Ethyl Acetate	348.2	1.23	1.16	-5.7%	1.15	-6.5%	[25]
1-Chlorobutane	N-Hexadecane	298.2	1.18	1.18	0.1%	1.07	-9.2%	[6]
1-Chlorobutane	N-Hexane	301.0	1.52	1.60	5.3%	1.29	-15.1%	[12]
1-Chlorobutane	N-Hexane	315.3	1.50	1.54	2.7%	1.25	-16.7%	[12]
1-Chlorobutane	N-Hexane	332.0	1.43	1.48	3.5%	1.21	-15.4%	[12]
1-Chlorobutane	N-Hexane	340.3	1.40	1.45	3.6%	1.19	-15.0%	[12]
1-Chlorobutane	Phenol	328.2	3.68	3.68	0.0%	M.P.	N.A.	[14]
1-Chlorobutane	Phenol	343.2	3.34	3.51	5.1%	M.P.	N.A.	[14]
1-Chlorobutane	Phenol	358.2	3.25	3.34	2.8%	M.P.	N.A.	[14]
1-Chlorobutane	Phenol	373.2	3.18	3.17	-0.3%	M.P.	N.A.	[14]
1-Chlorobutane	Tetraethylene Glycol DME	303.2	1.07	1.08	1.3%	1.00	-6.2%	[7]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Chlorobutane	Tetraethylene Glycol DME	323.2	1.05	1.05	-0.3%	0.98	-6.9%	[7]
1-Chlorobutane	Tetraethylene Glycol DME	343.2	1.10	1.03	-6.7%	0.95	-13.9%	[7]
1-Chlorobutane	Tributyl Phosphate	298.6	0.71	0.67	-5.6%	M.G.	N.A.	[27]
1-Chlorobutane	Tributyl Phosphate	302.9	0.73	0.67	-8.2%	M.G.	N.A.	[27]
1-Chlorobutane	Tributyl Phosphate	308.6	0.73	0.67	-8.2%	M.G.	N.A.	[27]
1-Chlorobutane	Tributyl Phosphate	313.1	0.75	0.67	-10.7%	M.G.	N.A.	[27]
1-Chlorobutane	Tributyl Phosphate	323.7	0.73	0.67	-8.2%	M.G.	N.A.	[27]
1-Chlorobutane	Tributyl Phosphate	330.0	0.69	0.67	-2.9%	M.G.	N.A.	[27]
1-Hexanol	1-Octanol	298.2	1.09	0.97	-11.0%	1.01	-7.3%	[3]
1-Hexanol	Carbon Tetrachloride	313.2	13.50	11.07	-18.0%	11.52	-14.7%	[28]
1-Hexanol	Carbon Tetrachloride	333.2	11.60	7.81	-32.7%	7.18	-38.1%	[28]
1-Hexanol	Cyclohexane	293.2	48.60	44.63	-8.2%	46.80	-3.7%	[28]
1-Hexanol	Cyclohexane	313.2	25.50	24.93	-2.2%	24.87	-2.5%	[28]
1-Hexanol	Cyclohexane	333.2	15.80	15.68	-0.8%	14.26	-9.7%	[28]
1-Hexanol	N-Hexadecane	298.2	22.82	29.42	28.9%	20.23	-11.3%	[6]
1-Hexanol	N-Hexane	293.2	45.40	38.58	-15.0%	36.30	-20.0%	[28]
1-Hexanol	N-Hexane	313.2	29.40	21.77	-26.0%	21.92	-25.4%	[28]
1-Hexanol	N-Hexane	333.2	19.80	13.81	-30.3%	14.15	-28.5%	[28]
1-Hexanol	Toluene	353.2	3.99	5.43	36.1%	3.27	-18.0%	[24]
1-Hexanol	Toluene	363.2	3.43	4.86	41.7%	2.93	-14.6%	[24]
1-Hexanol	Toluene	373.2	3.03	4.40	45.2%	2.67	-11.9%	[24]
1-Hexanol	Toluene	383.2	2.72	4.01	47.4%	2.49	-8.5%	[24]
1-Hexene	1,5-Dimethyl-2-Pyrrolidinone	298.2	4.76	5.23	9.9%	M.G.	N.A.	[29]
1-Hexene	1,5-Dimethyl-2-Pyrrolidinone	308.2	4.61	4.82	4.6%	M.G.	N.A.	[29]
1-Hexene	1,5-Dimethyl-2-Pyrrolidinone	318.2	4.56	4.48	-1.8%	M.G.	N.A.	[29]
1-Hexene	1-Butanol	308.2	4.41	4.39	-0.5%	3.94	-10.7%	[30]
1-Hexene	1-Butanol	318.2	4.03	4.26	5.7%	3.87	-4.0%	[30]
1-Hexene	1-Butanol	328.2	3.89	4.12	5.9%	3.79	-2.6%	[30]
1-Hexene	1-Ethylpyrrolidin-2-One	298.2	4.78	5.21	9.0%	2.55	-46.7%	[29]
1-Hexene	1-Ethylpyrrolidin-2-One	308.2	4.49	4.81	7.1%	2.52	-43.9%	[29]
1-Hexene	1-Ethylpyrrolidin-2-One	318.2	4.27	4.47	4.7%	2.49	-41.7%	[29]
1-Hexene	1-Octanol	293.4	2.43	2.55	4.9%	2.21	-9.1%	[31]
1-Hexene	1-Octanol	298.2	2.54	2.50	-1.6%	2.20	-13.4%	[32]
1-Hexene	1-Octanol	303.5	2.43	2.46	1.2%	2.18	-10.3%	[31]
1-Hexene	1-Octanol	313.6	2.29	2.37	3.5%	2.14	-6.6%	[31]
1-Hexene	1-Octanol	323.4	2.23	2.29	2.7%	2.11	-5.4%	[31]
1-Hexene	1-Pentanol	303.5	3.49	3.67	5.2%	3.24	-7.2%	[33]
1-Hexene	1-Pentanol	308.2	3.43	3.63	5.8%	3.21	-6.4%	[30]
1-Hexene	1-Pentanol	313.2	3.60	3.58	-0.6%	3.19	-11.4%	[33]
1-Hexene	1-Pentanol	318.2	3.23	3.52	9.0%	3.16	-2.2%	[30]
1-Hexene	1-Pentanol	323.5	3.45	3.47	0.6%	3.12	-9.6%	[33]
1-Hexene	1-Pentanol	328.2	3.48	3.41	-2.0%	3.09	-11.2%	[30]
1-Hexene	1-Phenyl-1-Butanone	298.1	2.56	2.82	10.2%	2.36	-7.8%	[34]
1-Hexene	2-Pyrrolidone	303.2	20.25	24.14	19.2%	M.G.	N.A.	[35]
1-Hexene	2-Pyrrolidone	313.2	19.37	20.73	7.0%	M.G.	N.A.	[35]
1-Hexene	2-Pyrrolidone	323.2	18.47	17.96	-2.8%	M.G.	N.A.	[35]
1-Hexene	2-Pyrrolidone	333.2	17.73	15.70	-11.4%	M.G.	N.A.	[35]
1-Hexene	Acetonitrile	298.2	12.70	15.38	21.1%	11.56	-9.0%	[36]
1-Hexene	Aniline	293.2	12.50	12.63	1.0%	13.43	7.4%	[37]
1-Hexene	Butanal	308.2	2.02	2.43	20.3%	2.10	4.2%	[38]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Hexene	Butanal	328.2	1.98	2.23	12.6%	2.00	1.1%	[38]
1-Hexene	Butanal	347.2	1.91	2.08	8.9%	1.92	0.3%	[38]
1-Hexene	Diethyl Phthalate	303.2	3.07	3.41	11.1%	M.G.	N.A.	[39]
1-Hexene	Diethyl Phthalate	313.2	2.94	3.19	8.5%	M.G.	N.A.	[39]
1-Hexene	Diethyl Phthalate	323.2	2.87	3.00	4.5%	M.G.	N.A.	[39]
1-Hexene	Diethyl Phthalate	333.2	2.78	2.84	2.2%	M.G.	N.A.	[39]
1-Hexene	Dimethyl Sulfoxide	283.2	42.00	40.06	-4.6%	34.65	-17.5%	[40]
1-Hexene	Epsilon-Caprolactone	303.2	7.24	7.87	8.7%	M.G.	N.A.	[41]
1-Hexene	Epsilon-Caprolactone	318.2	6.85	6.73	-1.8%	M.G.	N.A.	[41]
1-Hexene	Epsilon-Caprolactone	333.2	6.45	5.86	-9.1%	M.G.	N.A.	[41]
1-Hexene	Ethyl Benzoate	313.2	2.08	2.21	6.2%	M.G.	N.A.	[41]
1-Hexene	Ethyl Benzoate	323.2	2.05	2.13	3.9%	M.G.	N.A.	[41]
1-Hexene	Ethyl Benzoate	333.2	2.02	2.05	1.5%	M.G.	N.A.	[41]
1-Hexene	Ethyl Benzoate	343.2	1.99	1.99	0.0%	M.G.	N.A.	[41]
1-Hexene	Glutaronitrile	303.2	28.40	31.19	9.8%	M.G.	N.A.	[39]
1-Hexene	Glutaronitrile	313.2	26.10	25.87	-0.9%	M.G.	N.A.	[39]
1-Hexene	Glutaronitrile	323.2	24.40	21.77	-10.8%	M.G.	N.A.	[39]
1-Hexene	Glutaronitrile	333.2	22.70	18.57	-18.2%	M.G.	N.A.	[39]
1-Hexene	N,N-Diethylacetamide	303.2	3.20	3.60	12.5%	1.71	-46.6%	[39]
1-Hexene	N,N-Diethylacetamide	313.2	3.08	3.38	9.7%	1.69	-45.1%	[39]
1-Hexene	N,N-Diethylacetamide	323.2	2.97	3.18	7.1%	1.67	-43.8%	[39]
1-Hexene	N,N-Diethylacetamide	333.2	2.88	3.02	4.9%	1.65	-42.7%	[39]
1-Hexene	N,N-Dimethylformamide	283.2	11.30	11.88	5.1%	8.25	-27.0%	[40]
1-Hexene	N,N-Dimethylformamide	293.2	9.60	10.35	7.8%	7.76	-19.2%	[42]
1-Hexene	N,N-Dimethylformamide	313.2	7.70	8.10	5.2%	6.92	-10.1%	[42]
1-Hexene	N,N-Dimethylformamide	333.2	6.70	6.57	-1.9%	6.22	-7.2%	[42]
1-Hexene	N-Ethylacetamide	303.2	6.25	7.34	17.4%	M.G.	N.A.	[39]
1-Hexene	N-Ethylacetamide	313.2	6.17	6.96	12.8%	M.G.	N.A.	[39]
1-Hexene	N-Ethylacetamide	323.2	6.10	6.59	8.0%	M.G.	N.A.	[39]
1-Hexene	N-Ethylacetamide	333.2	6.03	6.23	3.3%	M.G.	N.A.	[39]
1-Hexene	N-Formylmorpholine	303.5	17.50	18.43	5.3%	M.G.	N.A.	[43]
1-Hexene	N-Formylmorpholine	323.2	14.50	14.02	-3.3%	M.G.	N.A.	[43]
1-Hexene	N-Formylmorpholine	342.8	11.90	11.06	-7.1%	M.G.	N.A.	[43]
1-Hexene	N-Methyl-2-Pyrrolidone	323.4	7.44	6.31	-15.2%	5.18	-30.4%	[43]
1-Hexene	N-Methyl-2-Pyrrolidone	333.2	6.86	5.82	-15.2%	5.08	-25.9%	[43]
1-Hexene	N-Methyl-2-Pyrrolidone	343.4	6.47	5.38	-16.8%	4.95	-23.5%	[43]
1-Hexene	N-Methylformamide	303.2	22.09	25.15	13.9%	M.P.	N.A.	[35]
1-Hexene	N-Methylformamide	313.2	21.11	22.66	7.3%	M.P.	N.A.	[35]
1-Hexene	N-Methylformamide	323.2	20.17	20.38	1.0%	M.P.	N.A.	[35]
1-Hexene	N-Methylformamide	333.2	19.44	18.32	-5.8%	M.P.	N.A.	[35]
1-Hexene	Phenol	328.2	9.24	9.15	-1.0%	6.51	-29.5%	[14]
1-Hexene	Phenol	343.2	8.30	8.38	1.0%	5.95	-28.3%	[14]
1-Hexene	Phenol	358.2	7.86	7.64	-2.8%	5.48	-30.3%	[14]
1-Hexene	Phenol	373.2	7.71	6.96	-9.7%	5.09	-34.0%	[14]
1-Hexene	Quinoline	293.2	5.56	5.43	-2.3%	M.G.	N.A.	[37]
1-Hexene	Sulfolane	303.2	29.50	24.09	-18.3%	M.G.	N.A.	[44]
1-Hexene	Sulfolane	313.2	26.60	20.17	-24.2%	M.G.	N.A.	[44]
1-Hexene	Toluene	293.2	1.46	1.56	6.8%	1.46	0.0%	[33]
1-Hexene	Toluene	293.2	1.44	1.56	8.3%	1.46	1.4%	[33]
1-Hexene	Toluene	293.2	1.36	1.56	14.7%	1.46	7.4%	[30]
1-Hexene	Toluene	303.2	1.43	1.52	6.3%	1.45	1.4%	[33]
1-Hexene	Toluene	303.2	1.33	1.52	14.3%	1.45	9.0%	[30]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Hexene	Toluene	313.2	1.55	1.49	-3.9%	1.44	-7.1%	[33]
1-Hexene	Toluene	313.2	1.30	1.49	14.6%	1.44	10.8%	[30]
1-Hexene	Tributyl Phosphate	298.6	1.39	1.48	6.5%	M.G.	N.A.	[27]
1-Hexene	Tributyl Phosphate	302.9	1.38	1.46	5.8%	M.G.	N.A.	[27]
1-Hexene	Tributyl Phosphate	308.6	1.35	1.43	5.9%	M.G.	N.A.	[27]
1-Hexene	Tributyl Phosphate	313.1	1.35	1.41	4.4%	M.G.	N.A.	[27]
1-Hexene	Tributyl Phosphate	323.7	1.28	1.36	6.3%	M.G.	N.A.	[27]
1-Hexene	Tributyl Phosphate	330.0	1.25	1.33	6.4%	M.G.	N.A.	[27]
1-Nitropropane	1-Octanol	298.2	6.43	6.44	0.2%	4.09	-36.4%	[3]
1-Nitropropane	Chlorobenzene	353.6	1.70	1.59	-6.5%	1.79	5.3%	[12]
1-Nitropropane	N-Hexadecane	298.2	10.31	11.21	8.7%	4.31	-58.2%	[6]
1-Nitropropane	N-Hexane	301.0	14.10	13.71	-2.8%	6.93	-50.9%	[12]
1-Nitropropane	N-Hexane	315.3	11.50	11.05	-3.9%	6.10	-47.0%	[12]
1-Nitropropane	N-Hexane	332.0	9.60	8.88	-7.5%	5.55	-42.2%	[12]
1-Nitropropane	N-Hexane	340.3	8.50	8.05	-5.3%	5.40	-36.5%	[12]
1-Nitropropane	Toluene	362.7	1.73	1.81	4.6%	1.49	-13.9%	[12]
1-Octanol	Butyronitrile	288.2	5.42	5.72	5.6%	2.53	-53.3%	23
1-Octanol	Butyronitrile	293.2	5.26	5.42	3.0%	2.49	-52.7%	23
1-Octanol	Butyronitrile	298.2	5.34	5.16	-3.3%	2.44	-54.3%	23
1-Octanol	Butyronitrile	303.2	4.45	4.92	10.6%	2.39	-46.3%	23
1-Octanol	Butyronitrile	308.2	4.23	4.70	11.1%	2.33	-44.9%	23
1-Octanol	Butyronitrile	313.2	3.93	4.50	14.5%	2.27	-42.2%	23
1-Octanol	Butyronitrile	323.2	3.64	4.14	13.9%	2.14	-41.1%	23
1-Octanol	Di-N-Propyl Ether	293.2	3.96	4.18	5.6%	3.17	-19.9%	338
1-Octanol	Di-N-Propyl Ether	298.2	3.69	3.96	7.3%	3.05	-17.4%	338
1-Octanol	Di-N-Propyl Ether	303.2	3.72	3.77	1.4%	2.94	-21.0%	338
1-Octanol	Di-N-Propyl Ether	308.2	3.50	3.59	2.5%	2.84	-19.0%	338
1-Octanol	Di-N-Propyl Ether	313.2	3.30	3.43	4.0%	2.75	-16.6%	338
1-Octanol	Di-N-Propyl Ether	323.2	3.05	3.16	3.7%	2.59	-15.0%	338
1-Octanol	Methyl Ethyl Ketone	293.2	2.85	2.65	-7.1%	2.60	-8.8%	76
1-Octanol	Methyl Ethyl Ketone	298.2	2.69	2.58	-4.2%	2.46	-8.6%	76
1-Octanol	Methyl Ethyl Ketone	303.2	2.38	2.51	5.5%	2.33	-2.1%	76
1-Octanol	Methyl Ethyl Ketone	308.2	2.44	2.45	0.3%	2.21	-9.5%	76
1-Octanol	Methyl Ethyl Ketone	313.2	2.35	2.39	1.9%	2.10	-10.5%	76
1-Octanol	Methyl Ethyl Ketone	323.2	2.23	2.28	2.4%	1.92	-13.7%	76
1-Octene	1,5-Dimethyl-2-Pyrrolidinone	298.2	6.04	7.26	20.2%	M.G.	N.A.	[29]
1-Octene	1,5-Dimethyl-2-Pyrrolidinone	308.2	6.00	6.57	9.5%	M.G.	N.A.	[29]
1-Octene	1,5-Dimethyl-2-Pyrrolidinone	318.2	5.95	6.00	0.8%	M.G.	N.A.	[29]
1-Octene	1-Ethylpyrrolidin-2-One	298.2	6.10	7.16	17.4%	3.32	-45.6%	[29]
1-Octene	1-Ethylpyrrolidin-2-One	308.2	5.80	6.50	12.1%	3.25	-44.0%	[29]
1-Octene	1-Ethylpyrrolidin-2-One	318.2	5.58	5.94	6.5%	3.17	-43.2%	[29]
1-Octene	1-Octanol	298.2	3.00	3.12	4.0%	2.66	-11.3%	[32]
1-Octene	1-Phenyl-1-Butanone	298.1	3.21	3.41	6.2%	3.05	-5.0%	[34]
1-Octene	2-Pyrrolidone	303.2	36.57	45.96	25.7%	M.G.	N.A.	[35]
1-Octene	2-Pyrrolidone	313.2	33.99	38.00	11.8%	M.G.	N.A.	[35]
1-Octene	2-Pyrrolidone	323.2	31.94	31.77	-0.5%	M.G.	N.A.	[35]
1-Octene	2-Pyrrolidone	333.2	30.13	26.86	-10.9%	M.G.	N.A.	[35]
1-Octene	Alpha-Pinene	353.2	1.15	1.23	7.0%	1.34	16.5%	[22]
1-Octene	Alpha-Pinene	373.2	1.10	1.21	10.0%	1.34	21.8%	[22]
1-Octene	Diethyl Phthalate	303.2	4.27	4.72	10.5%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Octene	Diethyl Phthalate	313.2	4.03	4.35	7.9%	M.G.	N.A.	[39]
1-Octene	Diethyl Phthalate	323.2	3.89	4.04	3.9%	M.G.	N.A.	[39]
1-Octene	Diethyl Phthalate	333.2	3.72	3.77	1.3%	M.G.	N.A.	[39]
1-Octene	Dimethyl Sulfoxide	283.2	89.50	90.11	0.7%	79.99	-10.6%	[40]
1-Octene	Epsilon-Caprolactone	303.2	11.10	12.05	8.6%	M.G.	N.A.	[41]
1-Octene	Epsilon-Caprolactone	318.2	10.20	9.92	-2.7%	M.G.	N.A.	[41]
1-Octene	Epsilon-Caprolactone	333.2	9.32	8.36	-10.3%	M.G.	N.A.	[41]
1-Octene	Ethyl Benzoate	313.2	2.32	2.54	9.5%	M.G.	N.A.	[41]
1-Octene	Ethyl Benzoate	323.2	2.26	2.43	7.5%	M.G.	N.A.	[41]
1-Octene	Ethyl Benzoate	333.2	2.22	2.33	5.0%	M.G.	N.A.	[41]
1-Octene	Ethyl Benzoate	343.2	2.18	2.24	2.8%	M.G.	N.A.	[41]
1-Octene	Glutaronitrile	303.2	65.80	69.26	5.3%	M.G.	N.A.	[39]
1-Octene	Glutaronitrile	313.2	59.00	54.75	-7.2%	M.G.	N.A.	[39]
1-Octene	Glutaronitrile	323.2	53.80	44.08	-18.1%	M.G.	N.A.	[39]
1-Octene	Glutaronitrile	333.2	48.90	36.09	-26.2%	M.G.	N.A.	[39]
1-Octene	N,N-Diethylacetamide	303.2	4.22	4.63	9.7%	1.85	-56.2%	[39]
1-Octene	N,N-Diethylacetamide	313.2	4.04	4.29	6.2%	1.81	-55.2%	[39]
1-Octene	N,N-Diethylacetamide	323.2	3.86	3.99	3.4%	1.77	-54.1%	[39]
1-Octene	N,N-Diethylacetamide	333.2	3.68	3.73	1.4%	1.74	-52.7%	[39]
1-Octene	N,N-Dimethylformamide	283.2	19.60	18.83	-3.9%	13.76	-29.8%	[40]
1-Octene	N,N-Dimethylformamide	293.2	15.50	15.85	2.3%	12.52	-19.2%	[42]
1-Octene	N,N-Dimethylformamide	313.2	12.60	11.69	-7.2%	10.49	-16.7%	[42]
1-Octene	N,N-Dimethylformamide	333.2	10.20	9.02	-11.6%	8.93	-12.5%	[42]
1-Octene	N-Ethylacetamide	303.2	9.06	10.36	14.3%	M.G.	N.A.	[39]
1-Octene	N-Ethylacetamide	313.2	9.00	9.71	7.9%	M.G.	N.A.	[39]
1-Octene	N-Ethylacetamide	323.2	8.97	9.09	1.3%	M.G.	N.A.	[39]
1-Octene	N-Ethylacetamide	333.2	8.89	8.48	-4.6%	M.G.	N.A.	[39]
1-Octene	N-Formylmorpholine	303.5	31.50	35.00	11.1%	M.G.	N.A.	[43]
1-Octene	N-Formylmorpholine	323.2	24.60	24.87	1.1%	M.G.	N.A.	[43]
1-Octene	N-Formylmorpholine	342.8	19.00	18.50	-2.6%	M.G.	N.A.	[43]
1-Octene	N-Methyl-2-Pyrrolidone	323.4	10.70	8.75	-18.2%	7.87	-26.4%	[43]
1-Octene	N-Methyl-2-Pyrrolidone	333.2	9.87	7.91	-19.9%	7.62	-22.8%	[43]
1-Octene	N-Methyl-2-Pyrrolidone	343.4	9.10	7.19	-21.0%	7.31	-19.7%	[43]
1-Octene	N-Methylformamide	303.2	40.30	44.89	11.4%	M.P.	N.A.	[35]
1-Octene	N-Methylformamide	313.2	38.18	39.43	3.3%	M.P.	N.A.	[35]
1-Octene	N-Methylformamide	323.2	36.22	34.56	-4.6%	M.P.	N.A.	[35]
1-Octene	N-Methylformamide	333.2	34.39	30.28	-12.0%	M.P.	N.A.	[35]
1-Octene	Phenol	328.2	12.23	12.43	1.6%	10.32	-15.6%	[14]
1-Octene	Phenol	343.2	10.65	11.20	5.2%	9.09	-14.6%	[14]
1-Octene	Phenol	358.2	9.77	10.04	2.8%	8.07	-17.4%	[14]
1-Octene	Phenol	373.2	9.33	8.99	-3.6%	7.22	-22.6%	[14]
1-Octene	Sulfolane	303.2	59.90	48.89	-18.4%	M.G.	N.A.	[44]
1-Octene	Sulfolane	313.2	53.60	39.13	-27.0%	M.G.	N.A.	[44]
1-Octene	Tributyl Phosphate	298.6	1.99	1.94	-2.5%	M.G.	N.A.	[27]
1-Octene	Tributyl Phosphate	302.9	1.72	1.90	10.5%	M.G.	N.A.	[27]
1-Octene	Tributyl Phosphate	308.6	1.68	1.86	10.7%	M.G.	N.A.	[27]
1-Octene	Tributyl Phosphate	313.1	1.68	1.82	8.3%	M.G.	N.A.	[27]
1-Octene	Tributyl Phosphate	330.0	1.52	1.71	12.5%	M.G.	N.A.	[27]
1-Pentanol	1-Octanol	298.2	1.09	0.98	-10.1%	1.03	-5.5%	[3]
1-Pentanol	Cyclohexane	312.9	22.11	21.57	-2.4%	28.34	28.2%	[17]
1-Pentanol	Cyclohexane	322.9	16.73	17.06	2.0%	21.22	26.8%	[17]
1-Pentanol	Cyclohexane	333.0	12.77	13.79	8.0%	16.13	26.3%	[17]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Pentanol	Cyclohexane	343.0	10.48	11.42	9.0%	12.53	19.6%	[17]
1-Pentanol	Cyclohexane	352.9	8.12	9.65	18.8%	9.93	22.3%	[17]
1-Pentanol	N-Hexadecane	298.2	27.10	23.98	-11.5%	21.90	-19.2%	[6]
1-Pentanol	N-Nonane	353.2	9.32	8.25	-11.5%	8.54	-8.4%	[21]
1-Pentanol	N-Nonane	373.2	5.61	6.17	10.0%	6.04	7.7%	[21]
1-Pentanol	Toluene	353.2	4.17	4.92	18.0%	3.75	-10.1%	[24]
1-Pentanol	Toluene	363.2	3.63	4.43	22.0%	3.34	-8.0%	[24]
1-Pentanol	Toluene	373.2	3.20	4.03	25.9%	3.05	-4.7%	[24]
1-Pentanol	Toluene	383.2	2.90	3.69	27.2%	2.83	-2.4%	[24]
1-Pentene	1,2-Dichloroethane	293.2	2.92	3.03	3.8%	1.89	-35.3%	[10]
1-Pentene	1,5-Dimethyl-2-Pyrrolidinone	298.2	4.06	4.21	3.7%	M.G.	N.A.	[29]
1-Pentene	1,5-Dimethyl-2-Pyrrolidinone	308.2	4.01	3.93	-2.0%	M.G.	N.A.	[29]
1-Pentene	1,5-Dimethyl-2-Pyrrolidinone	318.2	4.00	3.69	-7.8%	M.G.	N.A.	[29]
1-Pentene	1-Butanol	293.2	3.54	3.85	8.8%	3.51	-0.8%	[10]
1-Pentene	1-Ethylpyrrolidin-2-One	298.2	4.07	4.27	4.9%	2.21	-45.7%	[29]
1-Pentene	1-Ethylpyrrolidin-2-One	308.2	3.91	3.98	1.8%	2.20	-43.7%	[29]
1-Pentene	1-Ethylpyrrolidin-2-One	318.2	3.74	3.74	0.0%	2.18	-41.7%	[29]
1-Pentene	1-Octanol	293.4	2.25	2.21	-1.8%	1.99	-11.6%	[31]
1-Pentene	1-Octanol	303.5	2.26	2.14	-5.3%	1.96	-13.3%	[31]
1-Pentene	1-Octanol	313.6	2.16	2.08	-3.7%	1.93	-10.6%	[31]
1-Pentene	1-Octanol	323.4	2.12	2.01	-5.2%	1.90	-10.4%	[31]
1-Pentene	2,2,4-Trimethylpentane	293.2	0.99	0.95	-4.0%	1.01	2.0%	[10]
1-Pentene	2-Nitropropane	293.2	3.67	3.72	1.4%	2.84	-22.6%	[10]
1-Pentene	2-Pyrrolidone	303.2	16.07	16.37	1.9%	M.G.	N.A.	[35]
1-Pentene	2-Pyrrolidone	313.2	15.29	14.38	-6.0%	M.G.	N.A.	[35]
1-Pentene	2-Pyrrolidone	323.2	14.60	12.73	-12.8%	M.G.	N.A.	[35]
1-Pentene	2-Pyrrolidone	333.2	13.98	11.35	-18.8%	M.G.	N.A.	[35]
1-Pentene	Acetonitrile	293.2	13.80	10.48	-24.1%	9.29	-32.7%	[45]
1-Pentene	Acetonitrile	298.2	6.08	9.73	60.0%	8.98	47.7%	[36]
1-Pentene	Acetonitrile	313.2	11.29	7.94	-29.7%	8.13	-28.0%	[45]
1-Pentene	Acetophenone	293.2	3.68	3.64	-1.1%	4.22	14.7%	[10]
1-Pentene	Aniline	293.2	10.40	9.35	-10.1%	10.09	-3.0%	[10]
1-Pentene	Anisole	293.2	2.43	2.58	6.2%	1.72	-29.2%	[10]
1-Pentene	Benzene	293.2	1.72	1.81	5.2%	1.65	-4.1%	[10]
1-Pentene	Benzonitrile	293.2	3.62	3.58	-1.1%	M.G.	N.A.	[10]
1-Pentene	Cyclohexanone	293.2	2.59	2.63	1.5%	2.03	-21.6%	[10]
1-Pentene	Diethyl Phthalate	303.2	2.60	2.79	7.3%	M.G.	N.A.	[39]
1-Pentene	Diethyl Phthalate	313.2	2.51	2.64	5.2%	M.G.	N.A.	[39]
1-Pentene	Diethyl Phthalate	323.2	2.46	2.50	1.6%	M.G.	N.A.	[39]
1-Pentene	Diethyl Phthalate	333.2	2.39	2.38	-0.4%	M.G.	N.A.	[39]
1-Pentene	Epsilon-Caprolactone	303.2	5.85	5.96	1.9%	M.G.	N.A.	[41]
1-Pentene	Epsilon-Caprolactone	318.2	5.62	5.21	-7.3%	M.G.	N.A.	[41]
1-Pentene	Epsilon-Caprolactone	333.2	5.36	4.64	-13.4%	M.G.	N.A.	[41]
1-Pentene	Ethyl Acetate	293.2	2.05	2.18	6.3%	1.86	-9.3%	[10]
1-Pentene	Ethyl Benzoate	313.2	1.95	2.02	3.6%	M.G.	N.A.	[41]
1-Pentene	Ethyl Benzoate	323.2	1.92	1.96	2.1%	M.G.	N.A.	[41]
1-Pentene	Ethyl Benzoate	333.2	1.90	1.90	0.0%	M.G.	N.A.	[41]
1-Pentene	Ethyl Benzoate	343.2	1.88	1.84	-2.1%	M.G.	N.A.	[41]
1-Pentene	Methyl Ethyl Ketone	293.2	2.52	2.55	1.2%	2.38	-5.6%	[10]
1-Pentene	N,N-Diethylacetamide	303.2	2.79	2.96	6.1%	1.63	-41.6%	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Pentene	N,N-Diethylacetamide	313.2	2.71	2.80	3.3%	1.61	-40.6%	[39]
1-Pentene	N,N-Diethylacetamide	323.2	2.64	2.67	1.1%	1.60	-39.4%	[39]
1-Pentene	N,N-Diethylacetamide	333.2	2.56	2.55	-0.4%	1.59	-37.9%	[39]
1-Pentene	N,N-Dimethylformamide	293.2	7.00	7.67	9.6%	6.08	-13.1%	[42]
1-Pentene	N,N-Dimethylformamide	313.2	6.30	6.23	-1.1%	5.59	-11.3%	[42]
1-Pentene	N,N-Dimethylformamide	333.2	5.70	5.22	-8.4%	5.17	-9.3%	[42]
1-Pentene	N-Ethylacetamide	303.2	5.13	6.01	17.2%	M.G.	N.A.	[39]
1-Pentene	N-Ethylacetamide	313.2	5.06	5.74	13.4%	M.G.	N.A.	[39]
1-Pentene	N-Ethylacetamide	323.2	5.01	5.47	9.2%	M.G.	N.A.	[39]
1-Pentene	N-Ethylacetamide	333.2	4.97	5.20	4.6%	M.G.	N.A.	[39]
1-Pentene	N-Heptane	293.2	0.98	0.98	0.0%	1.03	5.1%	[10]
1-Pentene	Nitrobenzene	293.2	4.49	4.05	-9.8%	M.P.	N.A.	[10]
1-Pentene	Nitroethane	293.2	5.20	5.61	7.9%	3.99	-23.3%	[10]
1-Pentene	N-Methylformamide	303.2	16.40	17.42	6.2%	M.P.	N.A.	[35]
1-Pentene	N-Methylformamide	313.2	15.82	15.93	0.7%	M.P.	N.A.	[35]
1-Pentene	N-Methylformamide	323.2	15.24	14.54	-4.6%	M.P.	N.A.	[35]
1-Pentene	N-Methylformamide	333.2	14.68	13.27	-9.6%	M.P.	N.A.	[35]
1-Pentene	N-Octane	293.2	0.96	0.97	1.0%	1.01	5.2%	[10]
1-Pentene	Propionitrile	293.2	4.57	5.59	22.3%	4.24	-7.2%	[10]
1-Pentene	P-Xylene	293.2	1.24	1.32	6.5%	1.44	16.1%	[10]
1-Pentene	Toluene	293.2	1.44	1.60	11.1%	1.49	3.5%	[10]
1-Pentene	Tributyl Phosphate	298.6	1.27	1.20	-5.5%	M.G.	N.A.	[27]
1-Pentene	Tributyl Phosphate	302.9	1.34	1.18	-11.9%	M.G.	N.A.	[27]
1-Pentene	Tributyl Phosphate	308.6	1.22	1.16	-4.9%	M.G.	N.A.	[27]
1-Pentene	Tributyl Phosphate	313.1	1.26	1.15	-8.7%	M.G.	N.A.	[27]
1-Pentene	Tributyl Phosphate	323.7	1.17	1.12	-4.3%	M.G.	N.A.	[27]
1-Pentene	Tributyl Phosphate	330.0	1.16	1.10	-5.2%	M.G.	N.A.	[27]
1-Propanol	1-Butanol	313.2	1.04	0.97	-6.5%	1.01	-2.6%	3
1-Propanol	1-Butanol	333.2	1.02	0.97	-4.9%	1.01	-1.0%	[21]
1-Propanol	1-Butanol	353.2	1.02	0.97	-4.9%	1.01	-1.0%	[21]
1-Propanol	1-Octanol	293.4	1.11	1.01	-9.0%	1.11	0.0%	[31]
1-Propanol	1-Octanol	298.2	1.16	1.00	-13.8%	1.11	-4.3%	[3]
1-Propanol	1-Octanol	303.5	1.14	1.00	-12.3%	1.10	-3.5%	[31]
1-Propanol	1-Octanol	313.6	1.08	0.99	-8.3%	1.10	1.9%	[31]
1-Propanol	1-Octanol	323.4	1.06	0.98	-7.5%	1.10	3.8%	[31]
1-Propanol	2,2,4-Trimethylpentane	328.4	14.55	16.06	10.4%	18.33	26.0%	278
1-Propanol	2,2,4-Trimethylpentane	348.5	11.63	10.54	-9.4%	11.97	2.9%	278
1-Propanol	2,6-Dimethylpyridine	313.2	0.76	0.60	-21.4%	1.57	105.6%	168
1-Propanol	2-Methyl-1-Propanol	313.2	1.01	1.00	-0.8%	1.01	0.2%	15
1-Propanol	2-Methyl-2-Propanol	313.2	0.80	0.93	15.7%	1.25	55.5%	9
1-Propanol	Anisole	358.2	3.43	4.13	20.4%	2.54	-25.9%	49
1-Propanol	Anisole	368.2	3.18	3.78	18.8%	2.42	-24.0%	49
1-Propanol	Benzene	298.2	12.10	15.59	28.8%	16.92	39.8%	[46]
1-Propanol	Benzene	313.2	10.07	11.45	13.7%	11.34	12.6%	325
1-Propanol	Butyronitrile	278.2	4.03	3.76	-6.7%	1.66	-58.8%	29
1-Propanol	Butyronitrile	288.2	3.78	3.46	-8.4%	1.66	-56.0%	29
1-Propanol	Butyronitrile	293.2	3.57	3.33	-6.6%	1.65	-53.7%	29
1-Propanol	Butyronitrile	298.2	3.32	3.21	-3.4%	1.62	-51.3%	29
1-Propanol	Butyronitrile	303.2	3.20	3.10	-3.1%	1.59	-50.3%	29
1-Propanol	Butyronitrile	308.2	3.10	3.00	-3.3%	1.56	-49.7%	29
1-Propanol	Butyronitrile	313.2	2.94	2.90	-1.5%	1.53	-48.0%	29
1-Propanol	Butyronitrile	323.2	2.81	2.73	-2.9%	1.45	-48.4%	29

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Propanol	Carbon Tetrachloride	314.9	15.93	14.70	-7.7%	17.33	8.8%	[17]
1-Propanol	Carbon Tetrachloride	327.0	11.90	11.48	-3.5%	12.88	8.2%	[17]
1-Propanol	Carbon Tetrachloride	338.9	8.82	9.28	5.2%	9.90	12.2%	[17]
1-Propanol	Carbon Tetrachloride	344.4	8.78	8.48	-3.4%	8.85	0.8%	[17]
1-Propanol	Diethyl Phthalate	303.2	2.82	2.35	-16.7%	M.G.	N.A.	[39]
1-Propanol	Diethyl Phthalate	313.2	2.54	2.20	-13.4%	M.G.	N.A.	[39]
1-Propanol	Diethyl Phthalate	323.2	2.34	2.07	-11.5%	M.G.	N.A.	[39]
1-Propanol	Diethyl Phthalate	333.2	2.14	1.96	-8.4%	M.G.	N.A.	[39]
1-Propanol	Dimethyl Carbonate	313.2	4.73	4.64	-1.9%	M.G.	N.A.	249
1-Propanol	Di-N-Propyl Ether	278.2	6.25	7.88	26.1%	5.71	-8.7%	451
1-Propanol	Di-N-Propyl Ether	288.2	5.68	6.61	16.4%	5.24	-7.7%	451
1-Propanol	Di-N-Propyl Ether	293.2	5.43	6.10	12.3%	5.02	-7.6%	451
1-Propanol	Di-N-Propyl Ether	298.2	5.23	5.65	8.0%	4.83	-7.7%	451
1-Propanol	Di-N-Propyl Ether	303.2	5.16	5.26	2.0%	4.64	-10.0%	451
1-Propanol	Di-N-Propyl Ether	308.2	4.76	4.91	3.1%	4.47	-6.2%	451
1-Propanol	Di-N-Propyl Ether	313.2	4.69	4.61	-1.8%	4.31	-8.2%	451
1-Propanol	Di-N-Propyl Ether	323.2	4.28	4.09	-4.5%	4.02	-6.1%	451
1-Propanol	Epsilon-Caprolactone	303.2	2.10	1.68	-20.0%	M.G.	N.A.	[41]
1-Propanol	Epsilon-Caprolactone	318.2	1.89	1.64	-13.2%	M.G.	N.A.	[41]
1-Propanol	Epsilon-Caprolactone	333.2	1.67	1.61	-3.6%	M.G.	N.A.	[41]
1-Propanol	Ethanol	313.2	1.02	1.03	0.9%	1.02	0.0%	6
1-Propanol	Ethylene Glycol Ethyl Ether	313.2	1.14	1.05	-7.7%	0.96	-15.6%	383
1-Propanol	Glutaronitrile	303.2	5.46	5.65	3.5%	M.G.	N.A.	[39]
1-Propanol	Glutaronitrile	313.2	4.80	5.14	7.1%	M.G.	N.A.	[39]
1-Propanol	Glutaronitrile	323.2	4.31	4.71	9.3%	M.G.	N.A.	[39]
1-Propanol	Glutaronitrile	333.2	3.90	4.35	11.5%	M.G.	N.A.	[39]
1-Propanol	Methanol	313.2	1.13	1.21	7.4%	1.04	-7.7%	313
1-Propanol	Methanol	333.2	1.12	1.18	5.1%	1.04	-7.3%	313
1-Propanol	N,N-Dimethylformamide	313.2	0.80	0.57	-29.1%	0.76	-5.4%	67
1-Propanol	N-Decane	293.2	46.20	41.54	-10.1%	39.10	-15.4%	[23]
1-Propanol	N-Dodecane	293.2	44.40	40.16	-9.5%	35.53	-20.0%	[23]
1-Propanol	N-Formylmorpholine	323.2	1.56	1.43	-8.3%	M.G.	N.A.	[43]
1-Propanol	N-Formylmorpholine	342.8	1.46	1.38	-5.5%	M.G.	N.A.	[43]
1-Propanol	N-Heptane	303.2	30.79	31.94	3.7%	36.24	17.7%	309
1-Propanol	N-Heptane	313.2	25.68	23.91	-6.9%	28.17	9.7%	309
1-Propanol	N-Heptane	323.2	20.50	18.47	-9.9%	22.23	8.5%	309
1-Propanol	N-Heptane	333.2	16.49	14.66	-11.1%	17.78	7.8%	[21]
1-Propanol	N-Heptane	333.2	15.96	14.66	-8.1%	17.78	11.4%	[21]
1-Propanol	N-Heptane	353.2	8.95	9.87	10.3%	11.77	31.5%	[23]
1-Propanol	N-Hexadecane	293.2	37.70	37.10	-1.6%	30.48	-19.2%	[6]
1-Propanol	N-Hexadecane	298.2	31.55	31.21	-1.1%	26.60	-15.7%	[12]
1-Propanol	N-Hexane	301.0	39.00	35.02	-10.2%	42.01	7.7%	[12]
1-Propanol	N-Hexane	315.3	26.10	23.17	-11.2%	29.30	12.3%	[12]
1-Propanol	N-Hexane	331.8	16.60	15.52	-6.5%	20.06	20.8%	[12]
1-Propanol	N-Hexane	340.1	13.70	13.02	-5.0%	16.80	22.6%	[12]
1-Propanol	N-Methyl-2-Pyrrolidone	354.2	0.30	0.35	15.1%	0.37	21.7%	387
1-Propanol	N-Octane	293.2	48.00	43.27	-9.9%	44.03	-8.3%	[23]
1-Propanol	N-Octane	358.2	9.58	8.80	-8.2%	9.92	3.5%	336
1-Propanol	N-Octane	363.2	8.78	8.10	-7.8%	9.03	2.8%	336
1-Propanol	N-Tetradecane	293.2	38.90	38.54	-0.9%	32.75	-15.8%	[23]
1-Propanol	P-Xylene	313.2	9.99	12.60	26.1%	9.69	-3.0%	61
1-Propanol	Pyridine	313.2	1.08	0.76	-29.5%	0.71	-34.2%	184

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
1-Propanol	Toluene	293.2	15.90	17.47	9.9%	16.88	6.2%	[24]
1-Propanol	Toluene	303.2	13.70	13.87	1.2%	12.97	-5.3%	[24]
1-Propanol	Toluene	313.2	11.40	11.29	-1.0%	10.25	-10.1%	[24]
1-Propanol	Toluene	323.2	9.90	9.39	-5.2%	8.32	-16.0%	[24]
1-Propanol	Tributyl Phosphate	298.6	0.47	0.30	-36.2%	M.G.	N.A.	[27]
1-Propanol	Tributyl Phosphate	302.9	0.47	0.31	-34.0%	M.G.	N.A.	[27]
1-Propanol	Tributyl Phosphate	308.6	0.47	0.32	-31.9%	M.G.	N.A.	[27]
1-Propanol	Tributyl Phosphate	313.1	0.47	0.33	-29.8%	M.G.	N.A.	[27]
1-Propanol	Tributyl Phosphate	323.7	0.43	0.34	-20.9%	M.G.	N.A.	[27]
1-Propanol	Tributyl Phosphate	330.0	0.41	0.35	-14.6%	M.G.	N.A.	[27]
2,2,4-Trimethylpentane	1,2-Dichloroethane	343.5	3.43	4.83	40.8%	2.78	-19.0%	[12]
2,2,4-Trimethylpentane	1-Propanol	308.2	7.70	9.44	22.6%	8.38	8.8%	[47]
2,2,4-Trimethylpentane	1-Propanol	328.4	7.14	8.57	20.1%	7.68	7.6%	278
2,2,4-Trimethylpentane	1-Propanol	348.5	6.56	7.60	15.8%	6.82	3.9%	278
2,2,4-Trimethylpentane	Acetonitrile	293.2	82.43	55.32	-32.9%	47.36	-42.5%	286
2,2,4-Trimethylpentane	Acetonitrile	298.2	32.40	48.26	49.0%	41.96	29.5%	[36]
2,2,4-Trimethylpentane	Acetonitrile	313.2	52.75	33.13	-37.2%	29.80	-43.5%	286
2,2,4-Trimethylpentane	Aniline	293.2	39.43	56.45	43.2%	37.52	-4.8%	[37]
2,2,4-Trimethylpentane	Aniline	293.2	39.40	56.45	43.3%	37.52	-4.8%	[10]
2,2,4-Trimethylpentane	Benzene	313.2	2.26	2.71	20.2%	1.94	-14.0%	277
2,2,4-Trimethylpentane	Ethanol	296.7	14.00	18.28	30.6%	15.04	7.4%	[48]
2,2,4-Trimethylpentane	Ethanol	318.7	12.90	16.26	26.0%	13.43	4.1%	[48]
2,2,4-Trimethylpentane	Ethanol	333.2	12.13	14.64	20.7%	12.13	0.0%	63
2,2,4-Trimethylpentane	Ethanol	337.0	12.20	14.21	16.5%	11.77	-3.5%	[48]
2,2,4-Trimethylpentane	Ethanol	353.2	11.90	12.41	4.3%	10.14	-14.8%	[48]
2,2,4-Trimethylpentane	Isopropanol	308.2	7.48	7.78	4.0%	6.52	-12.8%	[47]
2,2,4-Trimethylpentane	Methyl Ethyl Ketone	293.2	4.79	5.65	17.9%	5.78	20.6%	58
2,2,4-Trimethylpentane	Methyl Ethyl Ketone	313.2	4.18	4.71	12.6%	4.90	17.2%	58
2,2,4-Trimethylpentane	Methyl Isobutyl Ketone	328.2	2.70	2.87	6.3%	2.88	6.7%	[49]
2,2,4-Trimethylpentane	Methyl Isobutyl Ketone	348.2	2.38	2.61	9.7%	2.63	10.5%	[49]
2,2,4-Trimethylpentane	Methyl Isobutyl Ketone	388.2	1.93	2.23	15.5%	2.24	16.1%	[49]
2,2,4-Trimethylpentane	N-Formylmorpholine	313.3	48.20	75.77	57.2%	M.G.	N.A.	[43]
2,2,4-Trimethylpentane	N-Formylmorpholine	332.7	36.00	51.01	41.7%	M.G.	N.A.	[43]
2,2,4-Trimethylpentane	N-Formylmorpholine	352.5	30.70	35.90	16.9%	M.G.	N.A.	[43]
2,2,4-Trimethylpentane	N-Formylmorpholine	373.4	24.40	26.01	6.6%	M.G.	N.A.	[43]
2,2,4-Trimethylpentane	Nitrobenzene	293.2	11.80	14.74	24.9%	10.95	-7.2%	[10]
2,2,4-Trimethylpentane	N-Methyl-2-Pyrrolidone	323.4	17.90	24.13	34.8%	13.62	-23.9%	[43]
2,2,4-Trimethylpentane	N-Methyl-2-Pyrrolidone	333.2	16.00	20.96	31.0%	12.77	-20.2%	[43]
2,2,4-Trimethylpentane	N-Methyl-2-Pyrrolidone	343.4	14.40	18.31	27.2%	11.89	-17.4%	[43]
2,2,4-Trimethylpentane	P-Xylene	313.2	1.57	1.79	14.3%	1.34	-14.4%	97
2,2,4-Trimethylpentane	Pyridine	293.2	10.75	11.49	6.9%	8.30	-22.8%	158
2,2,4-Trimethylpentane	Pyridine	298.2	9.80	10.73	9.5%	7.91	-19.3%	158
2,2,4-Trimethylpentane	Pyridine	303.2	8.88	10.05	13.2%	7.56	-14.8%	158
2,2,4-Trimethylpentane	Pyridine	308.2	8.30	9.44	13.7%	7.24	-12.8%	158
2,2,4-Trimethylpentane	Pyridine	313.2	7.82	8.88	13.5%	6.93	-11.4%	158
2,2,4-Trimethylpentane	Quinoline	293.2	12.92	16.73	29.5%	M.G.	N.A.	[37]
2,2,4-Trimethylpentane	Toluene	313.2	1.82	2.35	29.4%	1.52	-16.3%	99
2,2-Dimethylbutane	1-Propanol	308.2	6.00	7.12	18.7%	6.31	5.2%	[47]
2,2-Dimethylbutane	Acetonitrile	298.2	19.30	27.14	40.6%	25.89	34.1%	[36]
2,2-Dimethylbutane	Isopropanol	308.2	5.92	5.88	-0.7%	5.04	-14.9%	[47]
2,2-Dimethylpentane	Quinoline	293.2	11.42	12.20	6.8%	M.G.	N.A.	[37]
2,3,4-Trimethylpentane	1,2-Dichloroethane	298.2	5.61	5.69	1.4%	4.54	-19.1%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2,3,4-Trimethylpentane	1,4-Dioxane	298.2	7.68	6.46	-15.9%	7.54	-1.8%	[50]
2,3,4-Trimethylpentane	1-Butanol	298.2	5.93	6.71	13.2%	6.12	3.2%	[50]
2,3,4-Trimethylpentane	1-Hexene	298.2	1.17	0.98	-16.2%	1.03	-12.0%	[50]
2,3,4-Trimethylpentane	1-Octanol	298.2	3.05	3.55	16.4%	3.02	-1.0%	[50]
2,3,4-Trimethylpentane	1-Octene	298.2	1.07	1.02	-4.7%	1.05	-1.9%	[50]
2,3,4-Trimethylpentane	1-Propanol	298.2	8.05	8.80	9.3%	8.67	7.7%	[50]
2,3,4-Trimethylpentane	2,2,4-Trimethylpentane	298.2	1.08	1.05	-2.8%	1.00	-7.4%	[50]
2,3,4-Trimethylpentane	2-Heptanone	298.2	2.43	2.57	5.8%	2.85	17.3%	[50]
2,3,4-Trimethylpentane	2-Pentanone	298.2	3.29	3.76	14.3%	4.17	26.7%	[50]
2,3,4-Trimethylpentane	Acetic Acid	298.2	21.24	23.62	11.2%	19.18	-9.7%	[50]
2,3,4-Trimethylpentane	Acetone	298.2	8.71	8.37	-3.9%	8.29	-4.8%	[50]
2,3,4-Trimethylpentane	Acetonitrile	298.2	40.27	47.13	17.0%	42.17	4.7%	[50]
2,3,4-Trimethylpentane	Acetophenone	298.2	7.82	8.42	7.7%	13.79	76.3%	[50]
2,3,4-Trimethylpentane	Anisole	298.2	4.27	4.65	8.9%	3.23	-24.4%	[50]
2,3,4-Trimethylpentane	Benzene	298.2	2.26	2.29	1.3%	2.12	-6.2%	[50]
2,3,4-Trimethylpentane	Benzonitrile	298.2	7.90	9.10	15.2%	M.G.	N.A.	[50]
2,3,4-Trimethylpentane	Benzyl Alcohol	298.2	16.81	20.27	20.6%	14.21	-15.5%	[50]
2,3,4-Trimethylpentane	Butyl Acetate	298.2	2.37	2.52	6.3%	3.37	42.2%	[50]
2,3,4-Trimethylpentane	Butyronitrile	298.2	7.71	8.75	13.5%	7.87	2.1%	[50]
2,3,4-Trimethylpentane	Carbon Disulfide	298.2	2.46	2.53	2.8%	1.95	-20.7%	[50]
2,3,4-Trimethylpentane	Carbon Tetrachloride	298.2	1.36	1.34	-1.5%	1.24	-8.8%	[50]
2,3,4-Trimethylpentane	Chlorobenzene	298.2	2.34	2.43	3.8%	2.57	9.8%	[50]
2,3,4-Trimethylpentane	Chloroform	298.2	2.00	2.22	11.0%	1.99	-0.5%	[50]
2,3,4-Trimethylpentane	Cyclohexane	298.2	1.16	1.14	-1.7%	1.05	-9.5%	[50]
2,3,4-Trimethylpentane	Cyclohexanone	298.2	4.66	5.28	13.3%	3.63	-22.1%	[50]
2,3,4-Trimethylpentane	Dichloromethane	298.2	3.59	3.75	4.5%	3.54	-1.4%	[50]
2,3,4-Trimethylpentane	Dimethyl Sulfoxide	298.2	119.25	146.75	23.1%	159.60	33.8%	[50]
2,3,4-Trimethylpentane	Ethanol	298.2	13.35	17.17	28.6%	14.99	12.3%	[50]
2,3,4-Trimethylpentane	Ethyl Acetate	298.2	4.07	3.97	-2.5%	4.44	9.1%	[50]
2,3,4-Trimethylpentane	Isopropanol	298.2	8.27	8.16	-1.3%	6.74	-18.5%	[50]
2,3,4-Trimethylpentane	Methanol	298.2	37.16	47.44	27.7%	38.77	4.3%	[50]
2,3,4-Trimethylpentane	Methyl Acetate	298.2	6.89	6.97	1.2%	7.75	12.5%	[50]
2,3,4-Trimethylpentane	Methyl Ethyl Ketone	298.2	4.63	5.03	8.6%	5.55	19.9%	[50]
2,3,4-Trimethylpentane	N-Decane	298.2	1.01	1.02	1.0%	1.00	-1.0%	[50]
2,3,4-Trimethylpentane	N-Dodecane	298.2	1.01	1.02	1.0%	0.98	-3.0%	[50]
2,3,4-Trimethylpentane	N-Heptane	298.2	1.07	1.00	-6.5%	1.00	-6.5%	[50]
2,3,4-Trimethylpentane	N-Hexadecane	298.2	0.94	0.96	2.1%	0.94	0.0%	[50]
2,3,4-Trimethylpentane	N-Hexadecane	298.2	0.92	0.96	4.0%	0.94	1.8%	[6]
2,3,4-Trimethylpentane	N-Hexane	298.2	1.10	0.98	-10.9%	1.00	-9.1%	[50]
2,3,4-Trimethylpentane	Nitrobenzene	298.2	9.99	10.65	6.6%	10.52	5.3%	[50]
2,3,4-Trimethylpentane	Nitromethane	298.2	79.17	77.47	-2.1%	100.32	26.7%	[50]
2,3,4-Trimethylpentane	N-Methyl-2-Pyrrolidone	298.2	16.54	23.14	39.9%	15.71	-5.0%	[50]
2,3,4-Trimethylpentane	N-Methylformamide	298.2	56.82	79.82	40.5%	M.P.	N.A.	[50]
2,3,4-Trimethylpentane	N-Nonane	298.2	1.03	1.02	-1.0%	1.00	-2.9%	[50]
2,3,4-Trimethylpentane	N-Octane	298.2	1.06	1.01	-4.7%	1.00	-5.7%	[50]
2,3,4-Trimethylpentane	N-Pentane	298.2	1.22	0.97	-20.5%	1.00	-18.0%	[50]
2,3,4-Trimethylpentane	Propionitrile	298.2	14.37	17.54	22.1%	12.21	-15.0%	[50]
2,3,4-Trimethylpentane	P-Xylene	298.2	1.60	1.56	-2.5%	1.38	-13.8%	[50]
2,3,4-Trimethylpentane	Pyridine	298.2	7.85	8.18	4.2%	7.96	1.4%	[50]
2,3,4-Trimethylpentane	Squalane	298.2	0.68	0.64	-5.9%	0.78	14.7%	[50]
2,3,4-Trimethylpentane	Tetrahydrofuran	298.2	2.18	2.27	4.1%	1.95	-10.6%	[50]
2,3,4-Trimethylpentane	Toluene	298.2	1.86	1.96	5.4%	1.59	-14.5%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2,3,4-Trimethylpentane	Triethylamine	298.2	1.09	1.07	-1.8%	1.05	-3.7%	[50]
2,3-Dimethylbutane	Quinoline	293.2	9.43	9.12	-3.3%	M.G.	N.A.	[37]
2,4-Dimethylpentane	1,2-Dichloroethane	298.2	5.64	6.21	10.1%	4.01	-28.9%	[50]
2,4-Dimethylpentane	1,4-Dioxane	298.2	7.86	7.17	-8.8%	6.53	-16.9%	[50]
2,4-Dimethylpentane	1-Butanol	298.2	5.62	6.26	11.4%	5.43	-3.4%	[50]
2,4-Dimethylpentane	1-Hexene	298.2	1.22	1.04	-14.8%	1.05	-13.9%	[50]
2,4-Dimethylpentane	1-Octanol	298.2	3.02	3.41	12.9%	2.77	-8.3%	[50]
2,4-Dimethylpentane	1-Octene	298.2	1.07	1.09	1.9%	1.06	-0.9%	[50]
2,4-Dimethylpentane	1-Propanol	298.2	7.47	8.24	10.3%	7.51	0.5%	[50]
2,4-Dimethylpentane	1-Propanol	308.2	7.04	7.99	13.5%	7.30	3.7%	[47]
2,4-Dimethylpentane	2,2,4-Trimethylpentane	298.2	1.05	1.00	-4.8%	1.00	-4.8%	[50]
2,4-Dimethylpentane	2-Heptanone	298.2	2.39	2.46	2.9%	2.65	10.9%	[50]
2,4-Dimethylpentane	2-Pentanone	298.2	3.21	3.67	14.3%	3.78	17.8%	[50]
2,4-Dimethylpentane	Acetic Acid	298.2	19.26	21.18	10.0%	14.31	-25.7%	[50]
2,4-Dimethylpentane	Acetone	298.2	7.67	7.14	-6.9%	7.12	-7.2%	[50]
2,4-Dimethylpentane	Acetonitrile	298.2	33.61	37.12	10.4%	33.09	-1.5%	[50]
2,4-Dimethylpentane	Acetophenone	298.2	7.98	8.50	6.5%	11.38	42.6%	[50]
2,4-Dimethylpentane	Anisole	298.2	4.38	5.03	14.8%	3.00	-31.5%	[50]
2,4-Dimethylpentane	Benzene	298.2	2.42	2.64	9.1%	2.14	-11.6%	[50]
2,4-Dimethylpentane	Benzonitrile	298.2	7.87	8.70	10.5%	M.G.	N.A.	[50]
2,4-Dimethylpentane	Benzyl Alcohol	298.2	17.00	20.18	18.7%	11.93	-29.8%	[50]
2,4-Dimethylpentane	Butyl Acetate	298.2	2.30	2.52	9.6%	3.10	34.8%	[50]
2,4-Dimethylpentane	Butyronitrile	298.2	7.19	8.14	13.2%	6.53	-9.2%	[50]
2,4-Dimethylpentane	Carbon Disulfide	298.2	2.73	3.74	37.0%	2.27	-16.8%	[50]
2,4-Dimethylpentane	Carbon Tetrachloride	298.2	1.45	1.57	8.3%	1.29	-11.0%	[50]
2,4-Dimethylpentane	Chlorobenzene	298.2	2.49	2.78	11.6%	2.64	6.0%	[50]
2,4-Dimethylpentane	Chloroform	298.2	2.12	2.37	11.8%	1.99	-6.1%	[50]
2,4-Dimethylpentane	Cyclohexane	298.2	1.18	1.37	16.1%	1.07	-9.3%	[50]
2,4-Dimethylpentane	Cyclohexanone	298.2	4.62	5.36	16.0%	3.34	-27.7%	[50]
2,4-Dimethylpentane	Dichloromethane	298.2	3.60	4.03	11.9%	3.14	-12.8%	[50]
2,4-Dimethylpentane	Dimethyl Sulfoxide	298.2	95.88	127.98	33.5%	111.07	15.8%	[50]
2,4-Dimethylpentane	Ethanol	298.2	11.85	14.96	26.2%	12.43	4.9%	[50]
2,4-Dimethylpentane	Ethyl Acetate	298.2	3.81	3.71	-2.6%	3.83	0.5%	[50]
2,4-Dimethylpentane	Isopropanol	298.2	7.43	7.09	-4.6%	5.91	-20.5%	[50]
2,4-Dimethylpentane	Isopropanol	308.2	6.91	6.86	-0.7%	5.75	-16.8%	[47]
2,4-Dimethylpentane	Methanol	298.2	30.09	39.82	32.3%	29.63	-1.5%	[50]
2,4-Dimethylpentane	Methyl Acetate	298.2	6.31	5.93	-6.0%	6.22	-1.4%	[50]
2,4-Dimethylpentane	Methyl Ethyl Ketone	298.2	4.35	4.75	9.2%	4.92	13.1%	[50]
2,4-Dimethylpentane	N-Decane	298.2	1.04	1.09	4.8%	0.99	-4.8%	[50]
2,4-Dimethylpentane	N-Dodecane	298.2	1.07	1.11	3.7%	0.97	-9.3%	[50]
2,4-Dimethylpentane	N-Heptane	298.2	1.06	1.05	-0.9%	1.00	-5.7%	[50]
2,4-Dimethylpentane	N-Hexadecane	298.2	0.99	1.05	6.1%	0.92	-7.1%	[50]
2,4-Dimethylpentane	N-Hexadecane	298.2	0.98	1.05	7.5%	0.92	-5.8%	[6]
2,4-Dimethylpentane	N-Hexane	298.2	0.89	1.01	13.5%	1.00	12.4%	[50]
2,4-Dimethylpentane	Nitrobenzene	298.2	10.02	10.60	5.8%	9.09	-9.3%	[50]
2,4-Dimethylpentane	Nitromethane	298.2	61.59	57.80	-6.2%	70.01	13.7%	[50]
2,4-Dimethylpentane	N-Methyl-2-Pyrrolidone	298.2	16.11	24.99	55.1%	12.72	-21.0%	[50]
2,4-Dimethylpentane	N-Methylformamide	298.2	48.41	69.66	43.9%	M.P.	N.A.	[50]
2,4-Dimethylpentane	N-Nonane	298.2	1.04	1.09	4.8%	0.99	-4.8%	[50]
2,4-Dimethylpentane	N-Octane	298.2	1.07	1.07	0.0%	1.00	-6.5%	[50]
2,4-Dimethylpentane	N-Pentane	298.2	1.12	0.97	-13.4%	1.00	-10.7%	[50]
2,4-Dimethylpentane	Propionitrile	298.2	12.54	15.83	26.2%	10.62	-15.3%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2,4-Dimethylpentane	P-Xylene	298.2	1.66	1.72	3.6%	1.45	-12.7%	[50]
2,4-Dimethylpentane	Pyridine	298.2	7.88	8.59	9.0%	7.62	-3.3%	[50]
2,4-Dimethylpentane	Squalane	298.2	0.72	0.61	-15.3%	0.75	4.2%	[50]
2,4-Dimethylpentane	Tetrahydrofuran	298.2	2.16	2.45	13.4%	1.94	-10.2%	[50]
2,4-Dimethylpentane	Toluene	298.2	1.92	2.25	17.2%	1.65	-14.1%	[50]
2,4-Dimethylpentane	Triethylamine	298.2	1.08	1.06	-1.9%	1.05	-2.8%	[50]
2,5-Dimethylhexane	1,2-Dichloroethane	298.2	6.16	6.22	1.0%	4.54	-26.3%	[50]
2,5-Dimethylhexane	1,4-Dioxane	298.2	8.51	7.18	-15.6%	7.54	-11.4%	[50]
2,5-Dimethylhexane	1-Butanol	298.2	6.37	7.07	11.0%	6.12	-3.9%	[50]
2,5-Dimethylhexane	1-Hexene	298.2	1.15	0.98	-14.8%	1.03	-10.4%	[50]
2,5-Dimethylhexane	1-Octanol	298.2	3.38	3.75	10.9%	3.02	-10.7%	[50]
2,5-Dimethylhexane	1-Octene	298.2	1.09	1.04	-4.6%	1.05	-3.7%	[50]
2,5-Dimethylhexane	1-Propanol	298.2	8.61	9.34	8.5%	8.67	0.7%	[50]
2,5-Dimethylhexane	2,2,4-Trimethylpentane	298.2	1.06	1.03	-2.8%	1.00	-5.7%	[50]
2,5-Dimethylhexane	2-Heptanone	298.2	2.59	2.64	1.9%	2.85	10.0%	[50]
2,5-Dimethylhexane	2-Pentanone	298.2	3.50	3.92	12.0%	4.17	19.1%	[50]
2,5-Dimethylhexane	Acetic Acid	298.2	25.67	25.81	0.5%	19.18	-25.3%	[50]
2,5-Dimethylhexane	Acetone	298.2	9.38	8.57	-8.6%	8.29	-11.6%	[50]
2,5-Dimethylhexane	Acetonitrile	298.2	46.90	51.09	8.9%	42.17	-10.1%	[50]
2,5-Dimethylhexane	Acetophenone	298.2	9.35	9.35	0.0%	13.79	47.5%	[50]
2,5-Dimethylhexane	Anisole	298.2	4.77	5.09	6.7%	3.23	-32.3%	[50]
2,5-Dimethylhexane	Benzene	298.2	2.19	2.43	11.0%	2.12	-3.2%	[50]
2,5-Dimethylhexane	Benzonitrile	298.2	9.18	9.90	7.8%	M.G.	N.A.	[50]
2,5-Dimethylhexane	Benzyl Alcohol	298.2	21.60	23.43	8.5%	14.21	-34.2%	[50]
2,5-Dimethylhexane	Butyl Acetate	298.2	2.50	2.61	4.4%	3.37	34.8%	[50]
2,5-Dimethylhexane	Butyronitrile	298.2	8.51	9.33	9.6%	7.87	-7.5%	[50]
2,5-Dimethylhexane	Carbon Disulfide	298.2	2.51	2.89	15.1%	1.95	-22.3%	[50]
2,5-Dimethylhexane	Carbon Tetrachloride	298.2	1.38	1.39	0.7%	1.24	-10.1%	[50]
2,5-Dimethylhexane	Chlorobenzene	298.2	2.48	2.60	4.8%	2.57	3.6%	[50]
2,5-Dimethylhexane	Chloroform	298.2	2.07	2.29	10.6%	1.99	-3.9%	[50]
2,5-Dimethylhexane	Cyclohexane	298.2	1.20	1.19	-0.8%	1.05	-12.5%	[50]
2,5-Dimethylhexane	Cyclohexanone	298.2	5.09	5.68	11.6%	3.63	-28.7%	[50]
2,5-Dimethylhexane	Dichloromethane	298.2	3.78	3.94	4.2%	3.54	-6.3%	[50]
2,5-Dimethylhexane	Dimethyl Sulfoxide	298.2	153.28	178.50	16.5%	159.60	4.1%	[50]
2,5-Dimethylhexane	Ethanol	298.2	14.31	18.25	27.5%	14.99	4.8%	[50]
2,5-Dimethylhexane	Ethyl Acetate	298.2	4.33	4.07	-6.0%	4.44	2.5%	[50]
2,5-Dimethylhexane	Isopropanol	298.2	8.75	8.41	-3.9%	6.74	-23.0%	[50]
2,5-Dimethylhexane	Methanol	298.2	39.65	51.92	30.9%	38.77	-2.2%	[50]
2,5-Dimethylhexane	Methyl Acetate	298.2	7.50	7.08	-5.6%	7.75	3.3%	[50]
2,5-Dimethylhexane	Methyl Ethyl Ketone	298.2	4.88	5.23	7.2%	5.55	13.7%	[50]
2,5-Dimethylhexane	N-Decane	298.2	1.06	1.05	-0.9%	1.00	-5.7%	[50]
2,5-Dimethylhexane	N-Dodecane	298.2	1.09	1.07	-1.8%	0.98	-10.1%	[50]
2,5-Dimethylhexane	N-Heptane	298.2	1.11	1.01	-9.0%	1.00	-9.9%	[50]
2,5-Dimethylhexane	N-Hexadecane	298.2	1.02	1.02	0.0%	0.94	-7.8%	[50]
2,5-Dimethylhexane	N-Hexadecane	298.2	1.02	1.02	0.3%	0.94	-7.6%	[6]
2,5-Dimethylhexane	N-Hexane	298.2	1.07	0.98	-8.4%	1.00	-6.5%	[50]
2,5-Dimethylhexane	Nitrobenzene	298.2	11.90	11.85	-0.4%	10.52	-11.6%	[50]
2,5-Dimethylhexane	Nitromethane	298.2	96.23	84.96	-11.7%	100.32	4.3%	[50]
2,5-Dimethylhexane	N-Methyl-2-Pyrrolidone	298.2	20.21	27.61	36.6%	15.71	-22.3%	[50]
2,5-Dimethylhexane	N-Methylformamide	298.2	70.27	92.88	32.2%	M.P.	N.A.	[50]
2,5-Dimethylhexane	N-Nonane	298.2	1.06	1.05	-0.9%	1.00	-5.7%	[50]
2,5-Dimethylhexane	N-Octane	298.2	1.08	1.03	-4.6%	1.00	-7.4%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2,5-Dimethylhexane	N-Pentane	298.2	1.16	0.94	-19.0%	1.00	-13.8%	[50]
2,5-Dimethylhexane	Propionitrile	298.2	15.19	19.08	25.6%	12.21	-19.6%	[50]
2,5-Dimethylhexane	P-Xylene	298.2	1.66	1.62	-2.4%	1.38	-16.9%	[50]
2,5-Dimethylhexane	Pyridine	298.2	8.28	9.02	8.9%	7.96	-3.9%	[50]
2,5-Dimethylhexane	Squalane	298.2	0.77	0.65	-15.6%	0.78	1.3%	[50]
2,5-Dimethylhexane	Tetrahydrofuran	298.2	2.20	2.34	6.4%	1.95	-11.4%	[50]
2,5-Dimethylhexane	Toluene	298.2	1.91	2.08	8.9%	1.59	-16.8%	[50]
2,5-Dimethylhexane	Triethylamine	298.2	1.14	1.06	-7.0%	1.05	-7.9%	[50]
2,6-Dimethylpyridine	1-Butanol	313.2	0.59	0.94	58.1%	1.68	182.6%	166
2,6-Dimethylpyridine	1-Propanol	313.2	0.69	0.76	9.9%	2.16	212.3%	168
2,6-Dimethylpyridine	2-Butanol	313.2	0.86	0.95	10.8%	1.68	95.9%	165
2,6-Dimethylpyridine	2-Methyl-1-Propanol	313.2	0.66	0.98	49.4%	1.68	156.0%	187
2,6-Dimethylpyridine	2-Methyl-2-Propanol	313.2	1.34	1.06	-21.1%	1.91	42.2%	164
2,6-Dimethylpyridine	Ethanol	313.2	0.93	0.97	4.5%	3.16	240.6%	169
2,6-Dimethylpyridine	Isopropanol	313.2	1.12	1.08	-3.4%	2.11	88.7%	167
2,6-Dimethylpyridine	Methanol	313.2	0.98	0.81	-17.7%	4.19	325.6%	170
2-Butanol	1-Octanol	293.4	0.92	1.00	8.7%	1.06	15.2%	[31]
2-Butanol	1-Octanol	303.5	0.96	0.99	3.1%	1.06	10.4%	[31]
2-Butanol	1-Octanol	313.6	0.92	0.99	7.6%	1.06	15.2%	[31]
2-Butanol	1-Octanol	323.4	0.90	0.98	8.9%	1.05	16.7%	[31]
2-Butanol	2,6-Dimethylpyridine	313.2	0.90	0.72	-19.7%	1.34	49.5%	165
2-Butanol	Acetonitrile	333.2	3.64	3.82	5.0%	2.94	-19.2%	129
2-Butanol	Butyronitrile	278.2	4.49	3.92	-12.7%	1.76	-60.8%	26
2-Butanol	Butyronitrile	288.2	3.66	3.61	-1.2%	1.75	-52.1%	26
2-Butanol	Butyronitrile	293.2	3.41	3.47	1.9%	1.73	-49.2%	26
2-Butanol	Butyronitrile	298.2	3.13	3.35	7.2%	1.71	-45.3%	26
2-Butanol	Butyronitrile	303.2	3.09	3.23	4.5%	1.68	-45.6%	26
2-Butanol	Butyronitrile	308.2	2.90	3.13	7.8%	1.64	-43.5%	26
2-Butanol	Butyronitrile	313.2	2.72	3.03	11.3%	1.60	-41.2%	26
2-Butanol	Butyronitrile	323.2	2.48	2.86	15.5%	1.52	-38.6%	26
2-Butanol	Di-N-Propyl Ether	288.2	4.88	4.93	0.9%	4.65	-4.8%	71
2-Butanol	Di-N-Propyl Ether	293.2	4.55	4.62	1.5%	4.46	-2.0%	71
2-Butanol	Di-N-Propyl Ether	298.2	4.32	4.34	0.4%	4.29	-0.8%	71
2-Butanol	Di-N-Propyl Ether	303.2	4.17	4.09	-1.8%	4.13	-0.8%	71
2-Butanol	Di-N-Propyl Ether	308.2	3.80	3.87	1.8%	3.98	4.7%	71
2-Butanol	Methyl Ethyl Ketone	278.2	2.49	2.22	-10.9%	2.69	7.9%	68
2-Butanol	Methyl Ethyl Ketone	288.2	2.29	2.13	-7.2%	2.44	6.3%	68
2-Butanol	Methyl Ethyl Ketone	293.2	2.15	2.08	-3.0%	2.34	9.1%	68
2-Butanol	Methyl Ethyl Ketone	298.2	2.07	2.04	-1.4%	2.24	8.3%	68
2-Butanol	Methyl Ethyl Ketone	303.2	1.93	2.00	3.7%	2.16	12.0%	68
2-Butanol	Methyl Ethyl Ketone	308.2	1.88	1.97	4.6%	2.07	9.9%	68
2-Butanol	Methyl Ethyl Ketone	313.2	1.86	1.93	4.0%	2.00	7.8%	68
2-Butanol	Methyl Ethyl Ketone	323.2	1.70	1.87	9.8%	1.87	9.8%	68
2-Butanol	Pyridine	313.2	1.07	0.99	-7.5%	0.64	-40.2%	181
2-Butanone	Diiodomethane	298.2	3.90	1.46	-62.6%	M.G.	N.A.	[16]
2-Heptanone	1-Octanol	298.2	2.19	2.19	0.0%	2.05	-6.4%	[3]
2-Heptanone	N-Hexadecane	298.2	3.14	2.53	-19.4%	2.95	-6.0%	[6]
2-Methyl-1-Propanol	1-Butanol	313.2	1.01	1.02	1.1%	1.00	-0.9%	14
2-Methyl-1-Propanol	1-Octanol	298.2	1.21	1.05	-13.2%	1.06	-12.4%	[3]
2-Methyl-1-Propanol	1-Octanol	298.2	1.21	1.05	-13.2%	1.06	-12.4%	[3]
2-Methyl-1-Propanol	1-Propanol	313.2	1.01	1.00	-1.4%	1.01	-0.4%	15
2-Methyl-1-Propanol	2,6-Dimethylpyridine	313.2	1.35	0.75	-44.4%	1.34	-0.6%	187

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2-Methyl-1-Propanol	Acetonitrile	333.2	3.47	3.61	4.1%	2.94	-15.2%	128
2-Methyl-1-Propanol	Butyronitrile	278.2	5.77	4.02	-30.3%	1.76	-69.5%	25
2-Methyl-1-Propanol	Butyronitrile	288.2	4.23	3.69	-12.7%	1.75	-58.6%	25
2-Methyl-1-Propanol	Butyronitrile	293.2	3.58	3.54	-1.1%	1.73	-51.7%	25
2-Methyl-1-Propanol	Butyronitrile	298.2	3.45	3.41	-1.1%	1.71	-50.4%	25
2-Methyl-1-Propanol	Butyronitrile	303.2	3.25	3.29	1.2%	1.68	-48.3%	25
2-Methyl-1-Propanol	Butyronitrile	308.2	2.98	3.18	6.7%	1.64	-45.0%	25
2-Methyl-1-Propanol	Butyronitrile	313.2	2.87	3.08	7.5%	1.60	-44.2%	25
2-Methyl-1-Propanol	Butyronitrile	323.2	2.61	2.90	11.2%	1.52	-41.7%	25
2-Methyl-1-Propanol	Carbon Tetrachloride	293.2	18.50	16.80	-9.2%	27.19	47.0%	[51]
2-Methyl-1-Propanol	Diethyl Phthalate	298.2	2.36	2.66	12.7%	M.G.	N.A.	[52]
2-Methyl-1-Propanol	Diethyl Phthalate	348.2	1.68	2.02	20.2%	M.G.	N.A.	[52]
2-Methyl-1-Propanol	Di-N-Propyl Ether	278.2	5.31	6.58	23.9%	5.06	-4.7%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	288.2	4.54	5.63	24.0%	4.65	2.4%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	293.2	4.34	5.25	20.9%	4.46	2.7%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	298.2	4.17	4.90	17.6%	4.29	2.9%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	303.2	4.04	4.60	13.8%	4.13	2.2%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	308.2	3.83	4.33	13.0%	3.98	3.8%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	313.2	3.70	4.10	10.8%	3.84	3.7%	70
2-Methyl-1-Propanol	Di-N-Propyl Ether	323.2	3.47	3.69	6.3%	3.59	3.4%	70
2-Methyl-1-Propanol	Ethanol	313.2	1.07	1.07	0.3%	1.07	0.3%	16
2-Methyl-1-Propanol	Ethanol	351.4	1.22	1.06	-13.1%	1.05	-13.9%	[53]
2-Methyl-1-Propanol	Ethanol	351.5	1.22	1.06	-13.1%	1.05	-13.9%	[53]
2-Methyl-1-Propanol	Ethanol	424.0	1.38	1.02	-26.1%	1.00	-27.5%	[53]
2-Methyl-1-Propanol	Ethanol	424.0	1.38	1.02	-26.1%	1.00	-27.5%	[53]
2-Methyl-1-Propanol	Isopropanol	313.2	0.98	1.01	3.5%	1.02	4.6%	12
2-Methyl-1-Propanol	Methanol	313.2	1.25	1.24	-0.8%	1.16	-7.2%	17
2-Methyl-1-Propanol	Methyl Ethyl Ketone	278.2	2.48	2.28	-7.9%	2.69	8.6%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	288.2	2.19	2.18	-0.6%	2.44	11.2%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	293.2	2.15	2.13	-1.0%	2.34	8.7%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	298.2	2.00	2.08	3.9%	2.24	11.8%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	303.2	1.90	2.04	7.5%	2.16	13.8%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	308.2	1.90	2.00	5.5%	2.07	9.2%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	313.2	1.85	1.96	5.7%	2.00	7.8%	78
2-Methyl-1-Propanol	Methyl Ethyl Ketone	323.2	1.71	1.90	11.0%	1.87	9.2%	78
2-Methyl-1-Propanol	N,N-Dibutylformamide	318.3	0.63	0.63	0.3%	0.96	52.9%	[13]
2-Methyl-1-Propanol	N,N-Dibutylformamide	318.3	0.63	0.63	0.3%	0.96	52.9%	[13]
2-Methyl-1-Propanol	N,N-Dibutylformamide	332.4	0.66	0.66	0.8%	0.95	45.0%	[13]
2-Methyl-1-Propanol	N,N-Dibutylformamide	332.4	0.66	0.66	0.8%	0.95	45.0%	[13]
2-Methyl-1-Propanol	N,N-Dimethylacetamide	333.4	0.70	0.64	-8.8%	0.57	-18.8%	[13]
2-Methyl-1-Propanol	N,N-Dimethylacetamide	333.4	0.70	0.64	-8.8%	0.57	-18.8%	[13]
2-Methyl-1-Propanol	N-Heptane	298.2	32.50	26.97	-17.0%	36.27	11.6%	[54]
2-Methyl-1-Propanol	N-Hexadecane	298.2	27.00	23.95	-11.3%	23.95	-11.3%	[6]
2-Methyl-1-Propanol	N-Hexadecane	298.2	27.00	23.95	-11.3%	23.95	-11.3%	[6]
2-Methyl-1-Propanol	N-Hexadecane	303.2	18.19	20.73	14.0%	21.02	15.6%	[55]
2-Methyl-1-Propanol	N-Hexadecane	308.2	17.78	18.08	1.7%	18.53	4.2%	[55]
2-Methyl-1-Propanol	N-Hexadecane	313.2	15.33	15.90	3.7%	16.40	7.0%	[55]
2-Methyl-1-Propanol	N-Hexadecane	318.2	13.36	14.08	5.4%	14.57	9.1%	[55]
2-Methyl-1-Propanol	N-Hexadecane	323.2	11.70	12.55	7.3%	13.00	11.1%	[55]
2-Methyl-1-Propanol	N-Hexadecane	328.2	10.40	11.25	8.2%	11.63	11.8%	[55]
2-Methyl-1-Propanol	N-Methylacetamide	318.4	1.01	1.06	4.6%	1.00	-1.3%	[13]
2-Methyl-1-Propanol	N-Methylacetamide	318.4	1.01	1.06	4.6%	1.00	-1.3%	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2-Methyl-1-Propanol	N-Methylacetamide	333.2	0.97	1.04	7.2%	1.00	3.1%	[13]
2-Methyl-1-Propanol	N-Methylacetamide	333.2	0.97	1.04	7.2%	1.00	3.1%	[13]
2-Methyl-1-Propanol	N-Octane	293.2	46.00	31.04	-32.5%	38.70	-15.9%	[51]
2-Methyl-1-Propanol	P-Xylene	313.2	8.52	9.97	17.0%	8.08	-5.2%	380
2-Methyl-1-Propanol	Pyridine	313.2	1.14	1.00	-12.3%	0.64	-43.8%	180
2-Methyl-1-Propanol	Sulfolane	303.8	4.66	5.01	7.5%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Sulfolane	303.8	4.66	5.01	7.5%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Sulfolane	317.9	4.02	4.49	11.8%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Sulfolane	317.9	4.02	4.49	11.8%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Sulfolane	332.8	3.24	4.05	25.0%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Sulfolane	332.8	3.24	4.05	25.0%	M.G.	N.A.	[13]
2-Methyl-1-Propanol	Tetraethylene Glycol DME	303.2	1.13	0.88	-22.3%	1.09	-3.7%	[7]
2-Methyl-1-Propanol	Tetraethylene Glycol DME	323.2	1.03	0.90	-12.4%	0.97	-5.6%	[7]
2-Methyl-1-Propanol	Tetraethylene Glycol DME	343.2	0.95	0.91	-4.6%	0.92	-3.6%	[7]
2-Methyl-1-Propanol	Toluene	313.2	8.83	9.23	4.5%	8.63	-2.3%	22
2-Methyl-2-Propanol	1-Butanol	313.2	0.81	0.99	22.7%	1.20	48.7%	8
2-Methyl-2-Propanol	1-Octanol	298.2	0.88	1.07	21.6%	1.15	30.7%	[3]
2-Methyl-2-Propanol	1-Propanol	313.2	0.79	0.92	16.6%	1.27	61.0%	9
2-Methyl-2-Propanol	2,6-Dimethylpyridine	313.2	1.37	0.97	-29.4%	1.51	9.9%	164
2-Methyl-2-Propanol	Acetonitrile	333.2	2.59	3.03	17.0%	4.88	88.4%	127
2-Methyl-2-Propanol	Benzene	313.2	6.18	5.80	-6.1%	8.89	43.9%	20
2-Methyl-2-Propanol	Butyronitrile	298.2	2.86	3.13	9.3%	1.29	-55.0%	24
2-Methyl-2-Propanol	Butyronitrile	303.2	2.79	3.02	8.2%	1.27	-54.5%	24
2-Methyl-2-Propanol	Butyronitrile	308.2	2.64	2.92	10.8%	1.24	-52.9%	24
2-Methyl-2-Propanol	Butyronitrile	313.2	2.43	2.83	16.3%	1.21	-50.3%	24
2-Methyl-2-Propanol	Butyronitrile	318.2	2.34	2.75	17.4%	1.19	-49.2%	24
2-Methyl-2-Propanol	Butyronitrile	323.2	2.30	2.67	15.9%	1.16	-49.6%	24
2-Methyl-2-Propanol	Cyclohexane	318.2	11.33	13.05	15.2%	18.78	65.7%	155
2-Methyl-2-Propanol	Di-N-Propyl Ether	298.2	4.22	3.86	-8.5%	2.83	-32.9%	69
2-Methyl-2-Propanol	Di-N-Propyl Ether	303.2	4.08	3.66	-10.4%	2.73	-33.2%	69
2-Methyl-2-Propanol	Di-N-Propyl Ether	308.2	3.92	3.47	-11.4%	2.64	-32.6%	69
2-Methyl-2-Propanol	Di-N-Propyl Ether	313.2	3.64	3.30	-9.3%	2.56	-29.7%	69
2-Methyl-2-Propanol	Di-N-Propyl Ether	318.2	3.48	3.15	-9.5%	2.48	-28.7%	69
2-Methyl-2-Propanol	Di-N-Propyl Ether	323.2	3.33	3.02	-9.3%	2.40	-27.9%	69
2-Methyl-2-Propanol	Ethanol	313.2	0.78	1.02	30.8%	1.43	83.3%	10
2-Methyl-2-Propanol	Methanol	313.2	0.70	1.07	53.3%	1.53	119.2%	11
2-Methyl-2-Propanol	Methyl Ethyl Ketone	303.2	1.82	2.08	14.1%	2.12	16.3%	77
2-Methyl-2-Propanol	Methyl Ethyl Ketone	308.2	1.73	2.03	17.2%	2.04	17.8%	77
2-Methyl-2-Propanol	Methyl Ethyl Ketone	313.2	1.65	1.99	20.9%	1.97	19.7%	77
2-Methyl-2-Propanol	Methyl Ethyl Ketone	318.2	1.58	1.95	23.3%	1.91	20.7%	77
2-Methyl-2-Propanol	Methyl Ethyl Ketone	323.2	1.51	1.91	26.3%	1.85	22.3%	77
2-Methyl-2-Propanol	N-Formylmorpholine	303.5	2.35	2.61	11.1%	M.G.	N.A.	[43]
2-Methyl-2-Propanol	N-Formylmorpholine	323.2	1.89	2.38	25.9%	M.G.	N.A.	[43]
2-Methyl-2-Propanol	N-Formylmorpholine	342.8	1.75	2.21	26.3%	M.G.	N.A.	[43]
2-Methyl-2-Propanol	N-Heptane	313.2	9.57	11.62	21.4%	14.44	50.8%	1
2-Methyl-2-Propanol	N-Hexadecane	298.2	15.98	13.91	-13.0%	16.17	1.2%	[6]
2-Methyl-2-Propanol	N-Hexane	303.3	16.80	14.51	-13.6%	18.77	11.7%	[28]
2-Methyl-2-Propanol	N-Hexane	313.1	12.60	11.77	-6.6%	14.97	18.8%	[28]
2-Methyl-2-Propanol	N-Hexane	313.2	9.08	11.75	29.4%	14.93	64.4%	2
2-Methyl-2-Propanol	N-Hexane	322.8	9.51	9.78	2.8%	12.13	27.5%	[28]
2-Methyl-2-Propanol	N-Methyl-2-Pyrrolidone	323.4	0.80	0.83	3.4%	0.97	20.8%	[43]
2-Methyl-2-Propanol	N-Methyl-2-Pyrrolidone	333.2	0.80	0.87	8.6%	0.88	9.9%	[43]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2-Methyl-2-Propanol	N-Methyl-2-Pyrrolidone	343.4	0.83	0.91	9.1%	0.78	-6.5%	[43]
2-Methyl-2-Propanol	N-Octane	313.2	8.85	11.45	29.3%	14.00	58.1%	259
2-Methyl-2-Propanol	P-Xylene	313.2	7.20	6.36	-11.6%	8.06	12.0%	18
2-Methyl-2-Propanol	Pyridine	313.2	1.37	1.17	-14.9%	1.41	2.6%	179
2-Methyl-2-Propanol	Toluene	313.2	6.31	5.84	-7.4%	8.30	31.6%	19
2-Methylpentane	1,2-Dichloroethane	298.2	5.11	5.21	2.0%	3.54	-30.7%	[50]
2-Methylpentane	1,4-Dioxane	298.2	6.60	5.85	-11.4%	5.64	-14.5%	[50]
2-Methylpentane	1-Butanol	298.2	5.00	5.28	5.6%	4.80	-4.0%	[50]
2-Methylpentane	1-Hexene	298.2	1.07	1.04	-2.8%	1.06	-0.9%	[50]
2-Methylpentane	1-Octanol	298.2	2.66	2.91	9.4%	2.54	-4.5%	[50]
2-Methylpentane	1-Octene	298.2	1.04	1.05	1.0%	1.06	1.9%	[50]
2-Methylpentane	1-Propanol	298.2	6.47	6.86	6.0%	6.49	0.3%	[50]
2-Methylpentane	2,2,4-Trimethylpentane	298.2	1.01	0.99	-2.0%	1.00	-1.0%	[50]
2-Methylpentane	2-Heptanone	298.2	2.19	2.21	0.9%	2.45	11.9%	[50]
2-Methylpentane	2-Pentanone	298.2	2.95	3.23	9.5%	3.42	15.9%	[50]
2-Methylpentane	Acetic Acid	298.2	16.16	16.24	0.5%	10.70	-33.8%	[50]
2-Methylpentane	Acetone	298.2	6.89	6.14	-10.9%	6.11	-11.3%	[50]
2-Methylpentane	Acetonitrile	298.2	21.90	27.30	24.7%	26.03	18.9%	[36]
2-Methylpentane	Acetonitrile	298.2	25.22	27.30	8.2%	26.03	3.2%	[50]
2-Methylpentane	Acetophenone	298.2	6.57	6.64	1.1%	9.37	42.6%	[50]
2-Methylpentane	Anisole	298.2	3.87	4.19	8.3%	2.79	-27.9%	[50]
2-Methylpentane	Benzene	298.2	2.25	2.41	7.1%	2.16	-4.0%	[50]
2-Methylpentane	Benzonitrile	298.2	6.47	6.93	7.1%	M.G.	N.A.	[50]
2-Methylpentane	Benzyl Alcohol	298.2	12.84	14.40	12.1%	10.00	-22.1%	[50]
2-Methylpentane	Butyl Acetate	298.2	2.13	2.26	6.1%	2.84	33.3%	[50]
2-Methylpentane	Butyronitrile	298.2	6.24	6.68	7.1%	5.42	-13.1%	[50]
2-Methylpentane	Carbon Disulfide	298.2	2.39	3.29	37.7%	2.65	10.9%	[50]
2-Methylpentane	Carbon Tetrachloride	298.2	1.41	1.51	7.1%	1.33	-5.7%	[50]
2-Methylpentane	Chlorobenzene	298.2	2.33	2.49	6.9%	2.70	15.9%	[50]
2-Methylpentane	Chloroform	298.2	2.12	2.24	5.7%	1.99	-6.1%	[50]
2-Methylpentane	Cyclohexane	298.2	1.20	1.32	10.0%	1.09	-9.2%	[50]
2-Methylpentane	Cyclohexanone	298.2	4.21	4.49	6.7%	3.08	-26.8%	[50]
2-Methylpentane	Dichloromethane	298.2	3.51	3.65	4.0%	2.79	-20.5%	[50]
2-Methylpentane	Dimethyl Sulfoxide	298.2	60.38	77.23	27.9%	77.16	27.8%	[50]
2-Methylpentane	Ethanol	298.2	10.23	12.00	17.3%	10.31	0.8%	[50]
2-Methylpentane	Ethyl Acetate	298.2	3.44	3.31	-3.8%	3.30	-4.1%	[50]
2-Methylpentane	Ethyl Benzoate	313.2	3.00	3.27	9.0%	M.G.	N.A.	[41]
2-Methylpentane	Ethyl Benzoate	323.2	2.91	3.10	6.5%	M.G.	N.A.	[41]
2-Methylpentane	Ethyl Benzoate	333.2	2.85	2.95	3.5%	M.G.	N.A.	[41]
2-Methylpentane	Ethyl Benzoate	343.2	2.80	2.81	0.4%	M.G.	N.A.	[41]
2-Methylpentane	Isopropanol	298.2	6.49	6.06	-6.6%	5.18	-20.2%	[50]
2-Methylpentane	Methanol	298.2	23.90	29.56	23.7%	22.81	-4.6%	[50]
2-Methylpentane	Methyl Acetate	298.2	5.53	5.18	-6.3%	5.01	-9.4%	[50]
2-Methylpentane	Methyl Ethyl Ketone	298.2	4.00	4.14	3.5%	4.36	9.0%	[50]
2-Methylpentane	Methyl Tert-Butyl Ether	303.2	1.27	1.39	9.4%	1.26	-0.8%	[56]
2-Methylpentane	Methyl Tert-Butyl Ether	323.2	1.22	1.34	9.8%	1.22	0.0%	[56]
2-Methylpentane	N-Decane	298.2	1.00	1.03	3.0%	0.98	-2.0%	[50]
2-Methylpentane	N-Dodecane	298.2	1.02	1.02	0.0%	0.95	-6.9%	[50]
2-Methylpentane	N-Heptane	298.2	1.04	1.03	-1.0%	1.00	-3.8%	[50]
2-Methylpentane	N-Hexadecane	298.2	0.91	0.95	4.4%	0.90	-1.1%	[50]
2-Methylpentane	N-Hexadecane	298.2	0.89	0.95	6.4%	0.90	0.8%	[6]
2-Methylpentane	N-Hexane	298.2	1.00	1.01	1.0%	1.00	0.0%	[50]

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2-Methylpentane	Nitrobenzene	298.2	8.30	8.20	-1.2%	7.85	-5.4%	[50]
2-Methylpentane	Nitromethane	298.2	43.66	40.48	-7.3%	48.83	11.8%	[50]
2-Methylpentane	N-Methyl-2-Pyrrolidone	298.2	12.70	17.31	36.3%	10.26	-19.2%	[50]
2-Methylpentane	N-Methylformamide	298.2	34.48	46.20	34.0%	M.P.	N.A.	[50]
2-Methylpentane	N-Nonane	298.2	1.00	1.04	4.0%	0.99	-1.0%	[50]
2-Methylpentane	N-Octane	298.2	1.03	1.04	1.0%	0.99	-3.9%	[50]
2-Methylpentane	N-Pentane	298.2	0.98	0.99	1.0%	1.00	2.0%	[50]
2-Methylpentane	Propionitrile	298.2	10.35	12.30	18.8%	9.25	-10.6%	[50]
2-Methylpentane	P-Xylene	298.2	1.58	1.60	1.3%	1.52	-3.8%	[50]
2-Methylpentane	Pyridine	298.2	6.67	6.95	4.2%	7.30	9.4%	[50]
2-Methylpentane	Quinoline	293.2	9.41	9.13	-3.0%	M.G.	N.A.	[37]
2-Methylpentane	Squalane	298.2	0.65	0.56	-13.8%	0.72	10.8%	[50]
2-Methylpentane	Tetrahydrofuran	298.2	2.17	2.30	6.0%	1.93	-11.1%	[50]
2-Methylpentane	Toluene	298.2	1.83	2.06	12.6%	1.72	-6.0%	[50]
2-Methylpentane	Triethylamine	298.2	1.08	1.06	-1.9%	1.04	-3.7%	[50]
2-Nitropropane	Carbon Tetrachloride	314.9	4.58	4.24	-7.4%	3.56	-22.3%	[12]
2-Nitropropane	Carbon Tetrachloride	333.0	4.24	3.73	-12.0%	3.24	-23.6%	[12]
2-Nitropropane	Carbon Tetrachloride	340.2	4.10	3.56	-13.2%	3.12	-23.9%	[12]
2-Nitropropane	Carbon Tetrachloride	346.3	3.96	3.43	-13.4%	3.03	-23.5%	[12]
2-Nitropropane	Cyclohexane	337.9	8.15	8.73	7.1%	7.26	-10.9%	[12]
2-Nitropropane	Cyclohexane	346.1	7.40	7.98	7.8%	6.66	-10.0%	[12]
2-Nitropropane	Cyclohexane	351.7	6.87	7.53	9.6%	6.28	-8.6%	[12]
2-Pentanone	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.14	1.33	16.7%	M.G.	N.A.	[29]
2-Pentanone	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.20	1.32	10.0%	M.G.	N.A.	[29]
2-Pentanone	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.26	1.30	3.2%	M.G.	N.A.	[29]
2-Pentanone	1-Ethylpyrrolidin-2-One	298.2	1.26	1.35	7.1%	M.P.	N.A.	[29]
2-Pentanone	1-Ethylpyrrolidin-2-One	308.2	1.26	1.34	6.3%	M.P.	N.A.	[29]
2-Pentanone	1-Ethylpyrrolidin-2-One	318.2	1.21	1.32	9.1%	M.P.	N.A.	[29]
2-Pentanone	1-Octanol	298.2	2.17	2.07	-4.6%	2.06	-5.1%	[3]
2-Pentanone	2-Pyrrolidone	303.2	3.57	3.49	-2.3%	M.G.	N.A.	[35]
2-Pentanone	2-Pyrrolidone	313.2	3.52	3.30	-6.2%	M.G.	N.A.	[35]
2-Pentanone	2-Pyrrolidone	323.2	3.47	3.13	-9.8%	M.G.	N.A.	[35]
2-Pentanone	2-Pyrrolidone	333.2	3.42	2.97	-13.2%	M.G.	N.A.	[35]
2-Pentanone	Diethyl Phthalate	303.2	0.99	0.95	-3.9%	M.G.	N.A.	[39]
2-Pentanone	Diethyl Phthalate	313.2	0.99	0.94	-5.1%	M.G.	N.A.	[39]
2-Pentanone	Diethyl Phthalate	323.2	1.00	0.94	-6.0%	M.G.	N.A.	[39]
2-Pentanone	Diethyl Phthalate	333.2	1.01	0.94	-6.9%	M.G.	N.A.	[39]
2-Pentanone	Epsilon-Caprolactone	303.2	1.57	1.62	3.2%	M.G.	N.A.	[41]
2-Pentanone	Epsilon-Caprolactone	318.2	1.56	1.56	0.0%	M.G.	N.A.	[41]
2-Pentanone	Epsilon-Caprolactone	333.2	1.55	1.52	-1.9%	M.G.	N.A.	[41]
2-Pentanone	Glutaronitrile	303.2	2.50	2.70	8.0%	M.G.	N.A.	[39]
2-Pentanone	Glutaronitrile	313.2	2.47	2.56	3.6%	M.G.	N.A.	[39]
2-Pentanone	Glutaronitrile	323.2	2.45	2.43	-0.8%	M.G.	N.A.	[39]
2-Pentanone	Glutaronitrile	333.2	2.41	2.32	-3.7%	M.G.	N.A.	[39]
2-Pentanone	Methyl Isobutyl Ketone	328.2	1.08	1.01	-6.5%	1.01	-6.5%	[49]
2-Pentanone	Methyl Isobutyl Ketone	348.2	1.04	1.01	-2.9%	1.00	-3.8%	[49]
2-Pentanone	Methyl Isobutyl Ketone	388.2	1.00	1.01	1.0%	1.00	0.0%	[49]
2-Pentanone	N,N-Diethylacetamide	303.2	1.06	1.13	6.6%	0.82	-22.6%	[39]
2-Pentanone	N,N-Diethylacetamide	313.2	1.07	1.12	4.7%	0.83	-22.4%	[39]
2-Pentanone	N,N-Diethylacetamide	323.2	1.09	1.11	1.8%	0.84	-22.9%	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
2-Pentanone	N,N-Diethylacetamide	333.2	1.09	1.10	0.9%	0.85	-22.0%	[39]
2-Pentanone	N-Ethylacetamide	303.2	2.31	2.25	-2.6%	M.G.	N.A.	[39]
2-Pentanone	N-Ethylacetamide	313.2	2.25	2.21	-1.8%	M.G.	N.A.	[39]
2-Pentanone	N-Ethylacetamide	323.2	2.21	2.17	-1.8%	M.G.	N.A.	[39]
2-Pentanone	N-Ethylacetamide	333.2	2.17	2.13	-1.8%	M.G.	N.A.	[39]
2-Pentanone	N-Formylmorpholine	303.5	2.48	2.61	5.2%	M.G.	N.A.	[43]
2-Pentanone	N-Formylmorpholine	323.2	2.31	2.39	3.5%	M.G.	N.A.	[43]
2-Pentanone	N-Formylmorpholine	342.8	2.21	2.22	0.5%	M.G.	N.A.	[43]
2-Pentanone	N-Hexadecane	298.2	3.45	2.83	-18.0%	3.34	-3.2%	[6]
2-Pentanone	N-Methyl-2-Pyrrolidone	323.4	1.67	1.72	3.0%	M.P.	N.A.	[43]
2-Pentanone	N-Methyl-2-Pyrrolidone	333.2	1.64	1.68	2.4%	M.P.	N.A.	[43]
2-Pentanone	N-Methyl-2-Pyrrolidone	343.4	1.62	1.65	1.9%	M.P.	N.A.	[43]
2-Pentanone	N-Methylformamide	303.2	3.21	3.51	9.3%	M.P.	N.A.	[35]
2-Pentanone	N-Methylformamide	313.2	3.19	3.38	6.1%	M.P.	N.A.	[35]
2-Pentanone	N-Methylformamide	323.2	3.16	3.26	3.0%	M.P.	N.A.	[35]
2-Pentanone	N-Methylformamide	333.2	3.14	3.13	-0.4%	M.P.	N.A.	[35]
2-Pentanone	Tributyl Phosphate	298.6	0.82	0.69	-15.9%	M.G.	N.A.	[27]
2-Pentanone	Tributyl Phosphate	302.9	0.85	0.69	-18.8%	M.G.	N.A.	[27]
2-Pentanone	Tributyl Phosphate	308.6	0.85	0.69	-18.8%	M.G.	N.A.	[27]
2-Pentanone	Tributyl Phosphate	313.1	0.86	0.68	-20.9%	M.G.	N.A.	[27]
2-Pentanone	Tributyl Phosphate	323.7	0.84	0.68	-19.0%	M.G.	N.A.	[27]
3-Methylpentane	Acetonitrile	298.2	20.40	26.65	30.6%	26.03	27.6%	[36]
Acetaldehyde	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.04	1.04	0.0%	M.G.	N.A.	[29]
Acetaldehyde	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.08	1.03	-4.6%	M.G.	N.A.	[29]
Acetaldehyde	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.11	1.03	-7.2%	M.G.	N.A.	[29]
Acetaldehyde	1-Ethylpyrrolidin-2-One	298.2	1.08	1.08	0.0%	M.P.	N.A.	[29]
Acetaldehyde	1-Ethylpyrrolidin-2-One	308.2	1.13	1.07	-5.3%	M.P.	N.A.	[29]
Acetaldehyde	1-Ethylpyrrolidin-2-One	318.2	1.15	1.06	-7.8%	M.P.	N.A.	[29]
Acetaldehyde	Diethyl Phthalate	303.2	0.91	0.89	-1.8%	M.G.	N.A.	[39]
Acetaldehyde	Diethyl Phthalate	313.2	0.91	0.88	-2.8%	M.G.	N.A.	[39]
Acetaldehyde	Diethyl Phthalate	323.2	0.90	0.87	-3.7%	M.G.	N.A.	[39]
Acetaldehyde	Diethyl Phthalate	333.2	0.90	0.86	-4.6%	M.G.	N.A.	[39]
Acetaldehyde	Epsilon-Caprolactone	303.2	1.19	1.10	-7.6%	M.G.	N.A.	[41]
Acetaldehyde	Epsilon-Caprolactone	318.2	1.17	1.09	-6.8%	M.G.	N.A.	[41]
Acetaldehyde	Epsilon-Caprolactone	333.2	1.15	1.08	-6.1%	M.G.	N.A.	[41]
Acetaldehyde	Glutaronitrile	303.2	1.14	1.23	7.9%	M.G.	N.A.	[39]
Acetaldehyde	Glutaronitrile	313.2	1.14	1.21	6.1%	M.G.	N.A.	[39]
Acetaldehyde	Glutaronitrile	323.2	1.15	1.20	4.3%	M.G.	N.A.	[39]
Acetaldehyde	Glutaronitrile	333.2	1.15	1.18	2.6%	M.G.	N.A.	[39]
Acetaldehyde	N,N-Dibutylformamide	302.8	1.01	1.02	0.9%	1.06	4.8%	[13]
Acetaldehyde	N,N-Dibutylformamide	318.3	0.95	0.99	4.3%	1.08	13.8%	[13]
Acetaldehyde	N,N-Dibutylformamide	332.4	0.92	0.97	5.0%	1.10	19.0%	[13]
Acetaldehyde	N,N-Diethylacetamide	303.2	0.94	1.01	7.0%	M.P.	N.A.	[39]
Acetaldehyde	N,N-Diethylacetamide	313.2	0.95	1.00	5.2%	M.P.	N.A.	[39]
Acetaldehyde	N,N-Diethylacetamide	323.2	0.96	0.99	2.9%	M.P.	N.A.	[39]
Acetaldehyde	N,N-Diethylacetamide	333.2	0.97	0.98	1.4%	M.P.	N.A.	[39]
Acetaldehyde	N,N-Dimethylacetamide	303.2	0.94	1.04	10.6%	M.P.	N.A.	[13]
Acetaldehyde	N,N-Dimethylacetamide	317.6	0.91	1.04	14.0%	M.P.	N.A.	[13]
Acetaldehyde	N,N-Dimethylacetamide	333.4	0.88	1.03	16.8%	M.P.	N.A.	[13]
Acetaldehyde	N-Ethylacetamide	303.2	2.13	1.97	-7.5%	M.G.	N.A.	[39]

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Acetaldehyde	N-Ethylacetamide	313.2	2.02	1.93	-4.5%	M.G.	N.A.	[39]
Acetaldehyde	N-Ethylacetamide	323.2	1.98	1.89	-4.5%	M.G.	N.A.	[39]
Acetaldehyde	N-Ethylacetamide	333.2	1.91	1.85	-3.1%	M.G.	N.A.	[39]
Acetaldehyde	N-Methylacetamide	303.1	2.11	2.14	1.5%	M.P.	N.A.	[13]
Acetaldehyde	N-Methylacetamide	318.4	2.03	2.08	2.4%	M.P.	N.A.	[13]
Acetaldehyde	N-Methylacetamide	333.2	1.92	2.02	5.3%	M.P.	N.A.	[13]
Acetaldehyde	Sulfolane	303.1	1.44	1.38	-3.9%	M.G.	N.A.	[13]
Acetaldehyde	Sulfolane	317.9	1.38	1.34	-3.1%	M.G.	N.A.	[13]
Acetaldehyde	Sulfolane	333.6	1.33	1.30	-2.5%	M.G.	N.A.	[13]
Acetaldehyde	Tetraethylene Glycol DME	303.2	0.69	0.77	11.4%	0.80	15.8%	[7]
Acetaldehyde	Tetraethylene Glycol DME	323.2	0.70	0.76	8.4%	0.75	7.0%	[7]
Acetaldehyde	Tetraethylene Glycol DME	343.2	0.71	0.75	5.2%	0.71	-0.4%	[7]
Acetic Acid	1-Octanol	298.2	0.37	0.65	75.7%	1.62	337.8%	[3]
Acetic Acid	1-Octanol	298.2	0.37	0.65	75.7%	1.62	337.8%	[3]
Acetic Acid	Ethyl Acetate	313.2	1.22	1.17	-4.1%	1.59	30.3%	[57]
Acetic Acid	Ethyl Acetate	333.2	1.40	1.14	-18.6%	1.58	12.9%	[57]
Acetic Acid	Ethyl Acetate	353.2	1.57	1.11	-29.3%	1.57	0.0%	[57]
Acetic Acid	Ethyl Acetate	373.2	1.75	1.09	-37.7%	1.57	-10.3%	[57]
Acetic Acid	N-Heptane	313.2	24.66	40.14	62.8%	10.67	-56.7%	[57]
Acetic Acid	N-Heptane	333.2	18.86	22.69	20.3%	9.90	-47.5%	[57]
Acetic Acid	N-Heptane	353.2	18.11	14.30	-21.0%	9.40	-48.1%	[57]
Acetic Acid	N-Heptane	373.2	17.50	9.79	-44.1%	9.13	-47.8%	[57]
Acetone	1,2-Dichloroethane	293.2	0.76	0.79	3.9%	0.34	-55.3%	[10]
Acetone	1,2-Dichloroethane	318.5	0.76	0.85	11.8%	0.39	-48.7%	[12]
Acetone	1,2-Dichloroethane	337.2	0.78	0.88	12.8%	0.42	-46.2%	[12]
Acetone	1,2-Dichloroethane	354.7	0.78	0.91	16.7%	0.45	-42.3%	[12]
Acetone	1,2-Dichloroethane	356.7	0.89	0.91	2.2%	0.45	-49.4%	[11]
Acetone	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.05	1.19	13.3%	M.G.	N.A.	[29]
Acetone	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.10	1.18	7.3%	M.G.	N.A.	[29]
Acetone	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.15	1.17	1.7%	M.G.	N.A.	[29]
Acetone	1-Butanol	293.2	2.40	2.74	14.2%	2.45	2.1%	[10]
Acetone	1-Butanol	308.2	2.14	2.55	19.2%	2.15	0.5%	[30]
Acetone	1-Butanol	318.2	2.00	2.44	22.0%	1.99	-0.5%	[30]
Acetone	1-Butanol	328.2	1.83	2.34	27.9%	1.85	1.1%	[30]
Acetone	1-Chlorobutane	293.2	1.70	2.01	18.2%	1.44	-15.3%	[10]
Acetone	1-Chlorobutane	309.5	1.62	1.89	16.7%	1.42	-12.3%	[12]
Acetone	1-Chlorobutane	326.7	1.53	1.79	17.0%	1.41	-7.8%	[12]
Acetone	1-Chlorobutane	343.2	1.42	1.70	19.7%	1.39	-2.1%	[12]
Acetone	1-Chlorobutane	350.8	1.40	1.67	19.3%	1.38	-1.4%	[12]
Acetone	1-Ethylpyrrolidin-2-One	298.2	1.22	1.25	2.5%	M.P.	N.A.	[29]
Acetone	1-Ethylpyrrolidin-2-One	308.2	1.21	1.23	1.7%	M.P.	N.A.	[29]
Acetone	1-Ethylpyrrolidin-2-One	318.2	1.20	1.22	1.7%	M.P.	N.A.	[29]
Acetone	1-Octanol	293.2	2.57	3.11	21.0%	2.30	-10.5%	[10]
Acetone	1-Octanol	298.2	2.51	3.00	19.5%	2.18	-13.1%	[3]
Acetone	1-Pentanol	303.5	2.34	2.74	17.1%	2.20	-6.0%	[33]
Acetone	1-Pentanol	308.2	2.43	2.66	9.5%	2.11	-13.2%	[30]
Acetone	1-Pentanol	313.2	2.15	2.59	20.5%	2.02	-6.0%	[33]
Acetone	1-Pentanol	318.2	2.07	2.53	22.2%	1.94	-6.3%	[30]
Acetone	1-Pentanol	323.5	1.99	2.46	23.6%	1.86	-6.5%	[33]
Acetone	1-Pentanol	328.2	2.10	2.41	14.8%	1.79	-14.8%	[30]

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Acetone	1-Phenyl-1-Butanone	298.1	1.34	1.30	-3.0%	1.02	-23.9%	[34]
Acetone	2,2,4-Trimethylpentane	293.2	7.15	6.84	-4.3%	5.85	-18.2%	[10]
Acetone	2-Pyrrolidone	303.2	2.30	2.02	-12.3%	M.G.	N.A.	[35]
Acetone	2-Pyrrolidone	313.2	2.27	1.97	-13.0%	M.G.	N.A.	[35]
Acetone	2-Pyrrolidone	323.2	2.23	1.92	-13.9%	M.G.	N.A.	[35]
Acetone	2-Pyrrolidone	333.2	2.20	1.88	-14.4%	M.G.	N.A.	[35]
Acetone	Acetonitrile	293.2	1.10	1.02	-7.3%	1.11	0.9%	[10]
Acetone	Acetonitrile	298.2	1.04	1.02	-1.9%	1.11	6.7%	[36]
Acetone	Aniline	277.4	0.62	0.89	42.7%	0.62	-0.6%	370
Acetone	Aniline	293.2	0.80	0.89	11.3%	0.64	-20.0%	[10]
Acetone	Aniline	313.2	0.70	0.90	27.8%	0.72	2.2%	370
Acetone	Aniline	350.8	0.94	0.92	-2.5%	0.94	-0.3%	370
Acetone	Aniline	386.7	1.10	0.94	-14.8%	1.20	8.8%	370
Acetone	Benzene	293.2	1.73	1.69	-2.3%	1.44	-16.8%	[58]
Acetone	Benzene	293.2	1.71	1.69	-1.2%	1.44	-15.8%	[10]
Acetone	Benzene	323.2	1.63	1.60	-1.9%	1.45	-11.1%	268
Acetone	Benzene	332.2	1.63	1.57	-3.7%	1.44	-11.7%	[12]
Acetone	Benzene	349.8	1.62	1.53	-5.6%	1.43	-11.7%	[12]
Acetone	Benzene	350.7	1.60	1.53	-4.4%	1.43	-10.6%	[12]
Acetone	Benzene	353.3	1.52	1.53	0.7%	1.43	-5.9%	[11]
Acetone	Benzene	353.3	1.58	1.53	-3.2%	1.43	-9.5%	[11]
Acetone	Benzyl Acetate	298.2	1.12	1.03	-8.0%	1.02	-8.9%	[10]
Acetone	Carbon Disulfide	298.3	8.34	11.05	32.5%	7.35	-11.9%	[17]
Acetone	Carbon Disulfide	308.4	7.52	9.91	31.8%	6.93	-7.8%	[17]
Acetone	Carbon Disulfide	318.7	7.19	8.94	24.3%	6.54	-9.0%	[17]
Acetone	Carbon Tetrachloride	293.2	3.19	3.01	-5.6%	2.93	-8.2%	[10]
Acetone	Carbon Tetrachloride	295.7	3.15	2.97	-5.7%	2.90	-7.9%	[12]
Acetone	Carbon Tetrachloride	316.5	2.88	2.70	-6.2%	2.72	-5.6%	[12]
Acetone	Carbon Tetrachloride	328.9	2.82	2.56	-9.2%	2.61	-7.4%	[17]
Acetone	Carbon Tetrachloride	333.0	2.76	2.52	-8.7%	2.57	-6.9%	[12]
Acetone	Carbon Tetrachloride	338.6	2.68	2.47	-7.8%	2.51	-6.3%	[17]
Acetone	Carbon Tetrachloride	344.4	2.58	2.41	-6.6%	2.46	-4.7%	[17]
Acetone	Carbon Tetrachloride	346.8	2.59	2.39	-7.7%	2.44	-5.8%	[12]
Acetone	Carbon Tetrachloride	349.8	2.32	2.37	2.2%	2.41	3.9%	[11]
Acetone	Carbon Tetrachloride	349.8	1.93	2.37	22.8%	2.41	24.9%	[11]
Acetone	Chlorobenzene	313.2	1.56	1.74	11.3%	1.51	-3.4%	39
Acetone	Chlorobenzene	353.2	1.51	1.59	5.6%	1.54	2.3%	39
Acetone	Chlorobenzene	386.7	1.49	1.50	0.6%	1.49	0.0%	39
Acetone	Chloroform	305.0	0.39	0.32	-17.9%	0.34	-12.8%	[12]
Acetone	Chloroform	323.0	0.48	0.38	-20.8%	0.42	-12.5%	[12]
Acetone	Chloroform	323.2	0.37	0.38	1.6%	0.42	12.3%	213
Acetone	Chloroform	334.2	0.52	0.42	-19.2%	0.46	-11.5%	[11]
Acetone	Cyclohexane	323.2	5.77	7.09	22.8%	4.81	-16.7%	266
Acetone	Cyclohexanone	293.2	1.26	1.19	-5.6%	1.12	-11.1%	[10]
Acetone	Dichloromethane	298.2	0.69	0.51	-26.3%	0.45	-34.9%	221
Acetone	Dichloromethane	303.2	0.48	0.53	11.1%	0.46	-3.6%	221
Acetone	Dichloromethane	348.2	0.72	0.65	-9.9%	0.56	-22.4%	221
Acetone	Dichloromethane	398.2	0.77	0.75	-2.6%	0.66	-14.3%	221
Acetone	Diethyl Ether	298.1	2.27	2.25	-0.9%	2.27	0.0%	149
Acetone	Diethyl Ether	338.2	2.05	1.90	-7.2%	2.15	5.0%	149
Acetone	Diethyl Ether	388.3	1.87	1.64	-12.3%	1.95	4.3%	149
Acetone	Diethyl Phthalate	303.2	0.94	0.98	4.4%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Acetone	Diethyl Phthalate	313.2	0.94	0.97	3.5%	M.G.	N.A.	[39]
Acetone	Diethyl Phthalate	323.2	0.94	0.96	2.0%	M.G.	N.A.	[39]
Acetone	Diethyl Phthalate	333.2	0.94	0.95	1.0%	M.G.	N.A.	[39]
Acetone	Epsilon-Caprolactone	303.2	1.25	1.24	-0.8%	M.G.	N.A.	[41]
Acetone	Epsilon-Caprolactone	318.2	1.24	1.22	-1.6%	M.G.	N.A.	[41]
Acetone	Epsilon-Caprolactone	333.2	1.23	1.21	-1.6%	M.G.	N.A.	[41]
Acetone	Ethanol	293.2	2.38	2.50	5.0%	2.55	7.1%	[10]
Acetone	Ethanol	303.2	2.70	2.42	-10.4%	2.38	-11.9%	[18]
Acetone	Ethanol	313.2	2.50	2.35	-6.0%	2.23	-10.8%	[18]
Acetone	Ethanol	314.3	2.43	2.34	-3.7%	2.21	-9.1%	[18]
Acetone	Ethanol	318.5	2.35	2.31	-1.7%	2.16	-8.1%	[18]
Acetone	Ethanol	322.5	2.17	2.28	5.1%	2.11	-2.8%	[12]
Acetone	Ethanol	323.0	2.22	2.28	2.7%	2.10	-5.4%	[18]
Acetone	Ethanol	323.2	2.15	2.28	6.2%	2.10	-2.2%	215
Acetone	Ethanol	323.2	2.30	2.28	-0.9%	2.10	-8.7%	[18]
Acetone	Ethanol	335.8	2.03	2.19	7.9%	1.95	-3.9%	[12]
Acetone	Ethanol	348.3	1.92	2.12	10.4%	1.82	-5.2%	[12]
Acetone	Ethanol	351.5	1.73	2.10	21.4%	1.79	3.5%	[11]
Acetone	Ethyl Acetate	293.2	1.13	1.15	1.8%	1.10	-2.7%	[10]
Acetone	Glutaronitrile	303.2	1.25	1.22	-2.4%	M.G.	N.A.	[39]
Acetone	Glutaronitrile	313.2	1.25	1.20	-4.0%	M.G.	N.A.	[39]
Acetone	Glutaronitrile	323.2	1.26	1.19	-5.6%	M.G.	N.A.	[39]
Acetone	Glutaronitrile	333.2	1.26	1.18	-6.3%	M.G.	N.A.	[39]
Acetone	Methanol	298.2	2.16	2.07	-4.2%	2.06	-4.6%	[30]
Acetone	Methanol	303.2	2.11	2.05	-2.8%	2.03	-3.8%	[18]
Acetone	Methanol	308.2	2.04	2.02	-1.0%	2.00	-2.0%	[18]
Acetone	Methanol	313.2	2.00	2.00	0.0%	1.97	-1.5%	[18]
Acetone	Methanol	313.2	2.01	2.00	-0.5%	1.97	-2.0%	[18]
Acetone	Methanol	323.2	1.94	1.96	0.9%	1.91	-1.7%	214
Acetone	Methanol	337.7	1.72	1.90	10.5%	1.83	6.4%	[59]
Acetone	Methanol	337.8	1.98	1.90	-4.0%	1.83	-7.6%	[11]
Acetone	Methanol	337.8	1.83	1.90	3.8%	1.83	0.0%	[11]
Acetone	Methyl Ethyl Ketone	293.2	1.05	1.08	2.9%	1.01	-3.8%	[10]
Acetone	Methyl Isobutyl Ketone	328.2	1.23	1.28	4.1%	1.05	-14.6%	[49]
Acetone	Methyl Isobutyl Ketone	348.2	1.19	1.24	4.2%	1.04	-12.6%	[49]
Acetone	Methyl Isobutyl Ketone	388.2	1.11	1.19	7.2%	1.01	-9.0%	[49]
Acetone	N,N-Dibutylformamide	302.8	1.10	1.22	11.4%	1.17	6.8%	[13]
Acetone	N,N-Dibutylformamide	318.3	1.05	1.18	12.8%	1.16	10.9%	[13]
Acetone	N,N-Dibutylformamide	332.4	1.03	1.16	13.1%	1.15	12.1%	[13]
Acetone	N,N-Diethylacetamide	303.2	1.03	1.12	8.7%	0.97	-5.8%	[39]
Acetone	N,N-Diethylacetamide	313.2	1.03	1.11	7.8%	0.98	-4.9%	[39]
Acetone	N,N-Diethylacetamide	323.2	1.04	1.11	6.7%	0.98	-5.8%	[39]
Acetone	N,N-Diethylacetamide	333.2	1.04	1.10	5.8%	0.99	-4.8%	[39]
Acetone	N,N-Dimethylacetamide	303.6	1.10	1.15	4.8%	0.77	-29.8%	[13]
Acetone	N,N-Dimethylacetamide	317.6	1.03	1.14	10.6%	0.79	-23.4%	[13]
Acetone	N,N-Dimethylacetamide	333.4	0.97	1.13	17.0%	0.81	-16.1%	[13]
Acetone	N-Decane	313.2	3.83	5.61	46.3%	4.33	12.9%	317
Acetone	N-Decane	333.2	3.69	4.57	23.9%	3.63	-1.6%	317
Acetone	N-Ethylacetamide	303.2	2.07	2.18	5.3%	M.G.	N.A.	[39]
Acetone	N-Ethylacetamide	313.2	1.98	2.13	7.6%	M.G.	N.A.	[39]
Acetone	N-Ethylacetamide	323.2	1.93	2.08	7.8%	M.G.	N.A.	[39]
Acetone	N-Ethylacetamide	333.2	1.87	2.04	9.1%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Acetone	N-Formylmorpholine	303.5	1.57	1.51	-3.8%	M.G.	N.A.	[43]
Acetone	N-Formylmorpholine	323.2	1.52	1.46	-3.9%	M.G.	N.A.	[43]
Acetone	N-Formylmorpholine	342.8	1.48	1.41	-4.7%	M.G.	N.A.	[43]
Acetone	N-Heptane	273.2	8.96	10.16	13.4%	7.78	-13.2%	318
Acetone	N-Heptane	323.2	5.05	5.38	6.6%	4.65	-7.9%	318
Acetone	N-Heptane	323.2	5.10	5.38	5.5%	4.65	-8.8%	[18]
Acetone	N-Heptane	333.2	4.59	4.89	6.5%	4.27	-7.0%	[18]
Acetone	N-Heptane	343.2	4.27	4.47	4.7%	3.93	-8.0%	[18]
Acetone	N-Hexadecane	298.2	5.48	5.90	7.7%	3.99	-27.2%	[6]
Acetone	N-Hexadecane	333.2	3.69	3.96	7.3%	2.89	-21.7%	316
Acetone	N-Hexane	253.2	12.57	14.59	16.1%	10.80	-14.1%	217
Acetone	N-Hexane	268.2	10.95	11.12	1.6%	8.87	-19.0%	217
Acetone	N-Hexane	293.2	7.52	7.68	2.1%	6.66	-11.5%	217
Acetone	N-Hexane	301.5	6.21	6.92	11.4%	6.11	-1.6%	[18]
Acetone	N-Hexane	301.9	6.12	6.89	12.6%	6.09	-0.5%	[17]
Acetone	N-Hexane	303.4	6.17	6.77	9.7%	6.00	-2.8%	[18]
Acetone	N-Hexane	313.2	5.78	6.05	4.7%	5.46	-5.5%	[18]
Acetone	N-Hexane	318.2	5.28	5.74	8.8%	5.21	-1.3%	217
Acetone	N-Hexane	323.2	5.04	5.46	8.3%	4.98	-1.2%	[18]
Acetone	N-Hexane	333.2	4.55	4.96	9.0%	4.57	0.4%	[18]
Acetone	N-Hexane	342.0	3.91	4.59	17.4%	4.26	9.0%	[11]
Acetone	Nitrobenzene	293.2	1.24	0.97	-21.8%	1.24	0.0%	[10]
Acetone	Nitromethane	298.2	1.10	0.83	-24.4%	0.94	-14.4%	194
Acetone	Nitromethane	348.2	1.06	0.87	-18.2%	0.96	-9.7%	194
Acetone	N-Methyl-2-Pyrrolidone	323.4	1.32	1.52	15.2%	M.P.	N.A.	[43]
Acetone	N-Methyl-2-Pyrrolidone	333.2	1.29	1.50	16.3%	M.P.	N.A.	[43]
Acetone	N-Methyl-2-Pyrrolidone	343.4	1.29	1.48	14.7%	M.P.	N.A.	[43]
Acetone	N-Methylacetamide	303.4	2.10	2.27	8.2%	2.18	3.9%	[13]
Acetone	N-Methylacetamide	318.4	2.02	2.20	9.2%	2.07	2.7%	[13]
Acetone	N-Methylacetamide	333.2	1.92	2.14	11.6%	1.97	2.7%	[13]
Acetone	N-Methylformamide	303.2	2.14	2.09	-2.3%	M.P.	N.A.	[35]
Acetone	N-Methylformamide	313.2	2.11	2.05	-2.7%	M.P.	N.A.	[35]
Acetone	N-Methylformamide	323.2	2.08	2.01	-3.2%	M.P.	N.A.	[35]
Acetone	N-Methylformamide	333.2	2.05	1.97	-3.8%	M.P.	N.A.	[35]
Acetone	N-Octane	293.2	7.30	7.46	2.2%	5.85	-19.9%	[10]
Acetone	N-Octane	313.2	5.92	5.86	-1.0%	4.80	-18.9%	[36]
Acetone	N-Octane	333.2	5.79	4.78	-17.4%	4.02	-30.6%	[36]
Acetone	N-Pentane	238.2	19.07	20.02	5.0%	14.65	-23.2%	407
Acetone	N-Pentane	258.2	16.12	13.25	-17.8%	10.99	-31.8%	407
Acetone	N-Pentane	298.2	7.99	7.24	-9.4%	6.89	-13.8%	407
Acetone	N-Pentane	303.2	7.07	6.82	-3.5%	6.55	-7.4%	[18]
Acetone	P-Xylene	293.2	2.13	2.14	0.5%	2.16	1.4%	[10]
Acetone	Pyridine	303.2	1.25	1.46	16.5%	1.20	-4.2%	297
Acetone	Quinoline	298.2	1.50	1.43	-4.7%	M.G.	N.A.	[10]
Acetone	Sulfolane	303.8	1.62	1.56	-3.5%	M.G.	N.A.	[13]
Acetone	Sulfolane	317.9	1.54	1.51	-2.2%	M.G.	N.A.	[13]
Acetone	Sulfolane	334.2	1.47	1.47	0.3%	M.G.	N.A.	[13]
Acetone	Tetraethylene Glycol DME	323.2	0.85	0.90	6.1%	0.82	-3.3%	[7]
Acetone	Tetraethylene Glycol DME	343.2	0.83	0.89	7.2%	0.95	14.5%	[7]
Acetone	Toluene	293.2	1.95	1.95	0.0%	1.75	-10.3%	[33]
Acetone	Toluene	293.2	1.97	1.95	-1.0%	1.75	-11.2%	[33]
Acetone	Toluene	293.2	2.19	1.95	-11.0%	1.75	-20.1%	[30]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Acetone	Toluene	293.2	1.98	1.95	-1.5%	1.75	-11.6%	[10]
Acetone	Toluene	303.2	1.93	1.89	-2.1%	1.76	-8.8%	[33]
Acetone	Toluene	303.2	1.96	1.89	-3.6%	1.76	-10.2%	[30]
Acetone	Toluene	313.2	2.08	1.84	-11.5%	1.76	-15.4%	[33]
Acetone	Toluene	313.2	1.75	1.84	5.1%	1.76	0.6%	[30]
Acetone	Tributyl Phosphate	298.2	0.98	0.82	-16.3%	M.G.	N.A.	[20]
Acetone	Tributyl Phosphate	298.6	0.87	0.82	-5.7%	M.G.	N.A.	[27]
Acetone	Tributyl Phosphate	302.9	0.89	0.82	-7.9%	M.G.	N.A.	[27]
Acetone	Tributyl Phosphate	308.6	0.90	0.81	-10.0%	M.G.	N.A.	[27]
Acetone	Tributyl Phosphate	313.1	0.92	0.80	-13.0%	M.G.	N.A.	[27]
Acetone	Tributyl Phosphate	318.2	0.81	0.79	-2.5%	M.G.	N.A.	[20]
Acetone	Tributyl Phosphate	323.7	0.87	0.78	-10.3%	M.G.	N.A.	[27]
Acetone	Tributyl Phosphate	333.2	0.83	0.77	-7.2%	M.G.	N.A.	[20]
Acetonitrile	1,2-Dichloroethane	318.5	1.47	1.69	15.0%	0.70	-52.4%	[12]
Acetonitrile	1,2-Dichloroethane	333.2	1.46	1.63	11.4%	0.72	-50.8%	123
Acetonitrile	1,2-Dichloroethane	343.9	1.45	1.58	9.0%	0.72	-50.3%	[12]
Acetonitrile	1,2-Dichloroethane	355.9	1.43	1.54	7.7%	0.73	-49.0%	[12]
Acetonitrile	1,4-Dioxane	313.2	1.92	1.47	-23.5%	1.46	-24.0%	226
Acetonitrile	1-Butanol	293.2	5.67	5.19	-8.5%	5.46	-3.7%	[10]
Acetonitrile	1-Butanol	333.2	5.66	3.87	-31.6%	3.47	-38.7%	130
Acetonitrile	1-Chlorobutane	323.2	4.71	4.50	-4.5%	3.65	-22.5%	[25]
Acetonitrile	1-Chlorobutane	348.2	3.98	3.63	-8.8%	3.43	-13.8%	[25]
Acetonitrile	1-Octanol	293.2	7.48	6.75	-9.8%	6.44	-13.9%	[10]
Acetonitrile	1-Octanol	298.2	6.50	6.36	-2.2%	5.97	-8.2%	[3]
Acetonitrile	2,2,4-Trimethylpentane	293.2	54.57	29.33	-46.3%	30.64	-43.9%	286
Acetonitrile	2,2,4-Trimethylpentane	293.2	31.50	29.33	-6.9%	30.64	-2.7%	[10]
Acetonitrile	2,2,4-Trimethylpentane	313.2	33.28	18.86	-43.3%	21.69	-34.8%	286
Acetonitrile	2-Butanol	333.2	3.26	4.19	28.7%	3.47	6.6%	129
Acetonitrile	2-Methyl-1-Propanol	333.2	3.63	3.80	4.6%	3.47	-4.5%	128
Acetonitrile	2-Methyl-2-Propanol	333.2	2.89	3.20	10.9%	4.62	60.1%	127
Acetonitrile	Acetophenone	293.2	1.65	1.49	-9.7%	1.02	-38.2%	[10]
Acetonitrile	Aniline	293.2	0.98	1.10	12.3%	0.83	-15.3%	370
Acetonitrile	Aniline	343.2	1.03	1.07	4.1%	0.89	-13.4%	370
Acetonitrile	Aniline	393.2	1.10	1.05	-4.7%	0.96	-12.9%	370
Acetonitrile	Anisole	293.2	2.26	2.27	0.4%	1.30	-42.5%	[10]
Acetonitrile	Benzene	293.2	3.36	4.22	25.6%	2.86	-14.9%	[58]
Acetonitrile	Benzene	293.2	3.47	4.22	21.6%	2.86	-17.6%	[10]
Acetonitrile	Benzene	298.2	3.08	4.03	30.8%	2.83	-8.2%	190
Acetonitrile	Benzene	318.2	3.08	3.43	11.4%	2.72	-11.7%	[12]
Acetonitrile	Benzene	348.0	2.85	2.82	-1.1%	2.58	-9.5%	190
Acetonitrile	Benzene	397.9	2.64	2.23	-15.6%	2.40	-9.1%	190
Acetonitrile	Benzyl Acetate	298.2	1.51	1.51	0.0%	1.06	-29.8%	[10]
Acetonitrile	Carbon Tetrachloride	293.2	13.40	12.77	-4.7%	11.02	-17.8%	[10]
Acetonitrile	Carbon Tetrachloride	314.9	10.70	9.22	-13.8%	9.36	-12.5%	[12]
Acetonitrile	Carbon Tetrachloride	316.5	10.10	9.02	-10.7%	9.26	-8.3%	[12]
Acetonitrile	Carbon Tetrachloride	330.0	9.10	7.61	-16.4%	8.46	-7.0%	[12]
Acetonitrile	Carbon Tetrachloride	340.2	8.70	6.78	-22.1%	7.94	-8.7%	[12]
Acetonitrile	Carbon Tetrachloride	346.0	8.10	6.38	-21.2%	7.67	-5.3%	[12]
Acetonitrile	Chlorobenzene	293.2	3.52	4.10	16.3%	3.44	-2.4%	131
Acetonitrile	Chlorobenzene	328.2	3.23	3.08	-4.5%	3.15	-2.4%	131
Acetonitrile	Chlorobenzene	343.2	3.04	2.79	-8.3%	3.02	-0.7%	131
Acetonitrile	Chlorobenzene	393.2	2.69	2.18	-18.8%	2.62	-2.5%	131

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Acetonitrile	Chloroform	298.7	1.33	1.60	20.3%	1.21	-9.0%	[12]
Acetonitrile	Chloroform	318.3	1.27	1.55	22.0%	1.30	2.4%	[60]
Acetonitrile	Chloroform	319.8	1.32	1.55	17.4%	1.31	-0.8%	[12]
Acetonitrile	Chloroform	328.3	1.29	1.53	18.6%	1.35	4.7%	[60]
Acetonitrile	Chloroform	331.9	1.35	1.52	12.6%	1.36	0.7%	[12]
Acetonitrile	Cyclohexanone	293.2	1.43	1.34	-6.3%	1.40	-2.1%	[10]
Acetonitrile	Dichloromethane	298.2	1.14	1.51	32.1%	1.16	1.5%	223
Acetonitrile	Dichloromethane	348.2	1.27	1.40	10.1%	1.23	-3.3%	223
Acetonitrile	Dichloromethane	398.1	1.36	1.32	-2.9%	1.29	-5.1%	223
Acetonitrile	Diethyl Ether	298.1	3.97	5.01	26.3%	4.94	24.6%	148
Acetonitrile	Diethyl Ether	338.2	3.32	3.52	5.9%	3.74	12.5%	148
Acetonitrile	Diethyl Ether	388.2	2.67	2.59	-2.8%	2.78	4.3%	148
Acetonitrile	Ethanol	293.2	4.69	4.20	-10.4%	4.49	-4.2%	206
Acetonitrile	Ethanol	323.2	3.70	3.60	-2.6%	3.43	-7.2%	206
Acetonitrile	Ethanol	343.2	3.06	3.29	7.6%	2.96	-3.2%	206
Acetonitrile	Ethanol	393.2	2.09	2.70	29.2%	2.17	3.8%	206
Acetonitrile	Ethyl Acetate	311.7	1.73	1.66	-4.0%	1.36	-21.4%	[12]
Acetonitrile	Ethyl Acetate	313.2	1.52	1.65	8.5%	1.36	-10.6%	333
Acetonitrile	Ethyl Acetate	330.5	1.58	1.57	-0.6%	1.35	-14.6%	[12]
Acetonitrile	Ethyl Acetate	347.8	1.51	1.50	-0.7%	1.34	-11.3%	[12]
Acetonitrile	Ethyl Acetate	353.2	1.50	1.48	-1.2%	1.33	-11.2%	333
Acetonitrile	Ethyl Acetate	393.2	1.48	1.36	-8.0%	1.29	-12.7%	333
Acetonitrile	Methanol	326.0	2.66	2.97	11.8%	2.58	-2.9%	207
Acetonitrile	Methanol	333.5	2.60	2.90	11.7%	2.49	-4.1%	207
Acetonitrile	Methyl Ethyl Ketone	314.7	1.25	1.26	0.8%	1.13	-9.6%	[12]
Acetonitrile	Methyl Ethyl Ketone	333.3	1.25	1.23	-1.6%	1.13	-9.6%	[12]
Acetonitrile	Methyl Ethyl Ketone	333.7	1.18	1.23	4.3%	1.13	-4.2%	205
Acetonitrile	N,N-Dibutylformamide	302.8	1.17	1.34	14.9%	1.29	10.6%	[13]
Acetonitrile	N,N-Dibutylformamide	318.3	1.13	1.29	14.0%	1.21	6.9%	[13]
Acetonitrile	N,N-Dibutylformamide	332.4	1.12	1.25	11.8%	1.15	2.9%	[13]
Acetonitrile	N,N-Dimethylacetamide	303.2	0.69	0.66	-4.1%	M.P.	N.A.	[13]
Acetonitrile	N,N-Dimethylacetamide	317.6	0.69	0.69	-0.1%	M.P.	N.A.	[13]
Acetonitrile	N,N-Dimethylacetamide	333.4	0.69	0.72	3.7%	M.P.	N.A.	[13]
Acetonitrile	N-Heptane	293.2	30.00	31.55	5.2%	33.64	12.1%	[10]
Acetonitrile	N-Hexadecane	298.2	24.30	24.42	0.5%	17.66	-27.3%	[6]
Acetonitrile	N-Hexane	295.0	27.60	30.55	10.7%	36.36	31.7%	[12]
Acetonitrile	N-Hexane	322.9	16.80	17.10	1.8%	22.77	35.5%	[12]
Acetonitrile	N-Hexane	330.9	12.40	14.86	19.8%	20.14	62.4%	[12]
Acetonitrile	N-Hexane	332.3	13.70	14.51	5.9%	19.73	44.0%	[12]
Acetonitrile	Nitrobenzene	293.2	1.73	1.48	-14.5%	M.P.	N.A.	[10]
Acetonitrile	Nitromethane	298.2	1.07	0.98	-8.4%	0.96	-10.3%	192
Acetonitrile	Nitromethane	348.2	1.01	0.99	-2.4%	0.97	-4.4%	192
Acetonitrile	Nitromethane	398.2	1.04	0.99	-5.1%	0.96	-7.9%	192
Acetonitrile	N-Methylacetamide	303.1	2.14	1.87	-12.5%	M.P.	N.A.	[13]
Acetonitrile	N-Methylacetamide	318.4	2.02	1.81	-10.3%	M.P.	N.A.	[13]
Acetonitrile	N-Methylacetamide	333.2	1.93	1.75	-9.2%	M.P.	N.A.	[13]
Acetonitrile	N-Octane	293.2	31.30	31.09	-0.7%	30.67	-2.0%	[10]
Acetonitrile	N-Octane	313.2	26.10	19.93	-23.6%	21.71	-16.8%	[36]
Acetonitrile	N-Octane	333.2	18.30	13.78	-24.7%	15.89	-13.2%	[36]
Acetonitrile	P-Xylene	293.2	5.05	6.12	21.2%	4.49	-11.1%	[10]
Acetonitrile	Quinoline	298.2	2.14	1.56	-27.1%	M.G.	N.A.	[10]
Acetonitrile	Sulfolane	303.8	1.06	1.02	-4.0%	M.G.	N.A.	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Acetonitrile	Sulfolane	317.9	1.07	1.02	-4.7%	M.G.	N.A.	[13]
Acetonitrile	Sulfolane	334.2	1.08	1.01	-6.2%	M.G.	N.A.	[13]
Acetonitrile	Tetraethylene Glycol DME	303.2	0.56	0.91	63.7%	0.50	-10.1%	[7]
Acetonitrile	Tetraethylene Glycol DME	323.2	0.63	0.90	43.5%	0.50	-20.3%	[7]
Acetonitrile	Tetraethylene Glycol DME	343.2	0.67	0.88	31.9%	0.48	-28.0%	[7]
Acetonitrile	Toluene	293.2	3.76	5.20	38.4%	3.58	-4.7%	334
Acetonitrile	Toluene	293.2	4.00	5.20	30.0%	3.58	-10.5%	[10]
Acetonitrile	Toluene	343.2	3.46	3.33	-3.8%	3.19	-7.9%	334
Acetonitrile	Toluene	393.2	2.96	2.49	-15.9%	2.92	-1.4%	334
Acetonitrile	Tributyl Phosphate	298.6	0.93	1.03	10.8%	M.G.	N.A.	[27]
Acetonitrile	Tributyl Phosphate	302.9	0.97	1.02	5.2%	M.G.	N.A.	[27]
Acetonitrile	Tributyl Phosphate	308.6	0.91	1.00	9.9%	M.G.	N.A.	[27]
Acetonitrile	Tributyl Phosphate	313.1	0.91	0.99	8.8%	M.G.	N.A.	[27]
Acetonitrile	Tributyl Phosphate	323.7	0.89	0.96	7.9%	M.G.	N.A.	[27]
Acetonitrile	Tributyl Phosphate	330.0	0.84	0.94	11.9%	M.G.	N.A.	[27]
Acetonitrile	Triethylamine	348.7	5.50	5.25	-4.5%	M.P.	N.A.	[12]
Acetophenone	Benzyl Alcohol	413.2	1.10	0.98	-10.6%	0.90	-17.9%	324
Acetophenone	Benzyl Alcohol	473.2	1.02	0.98	-4.0%	0.61	-40.2%	324
Alpha-Pinene	1-Butanol	353.2	6.42	5.78	-10.0%	3.37	-47.5%	[22]
Alpha-Pinene	1-Butanol	373.2	5.08	5.17	1.8%	3.09	-39.2%	[22]
Alpha-Pinene	1-Octene	353.2	1.22	1.23	0.8%	1.36	11.5%	[22]
Alpha-Pinene	1-Octene	373.2	1.14	1.21	6.1%	1.36	19.3%	[22]
Alpha-Pinene	Anisole	353.2	2.19	2.38	8.7%	1.91	-12.8%	[22]
Alpha-Pinene	Anisole	373.2	1.98	2.19	10.6%	1.73	-12.6%	[22]
Alpha-Pinene	Benzene	338.2	1.76	1.42	-19.3%	1.36	-22.7%	[22]
Alpha-Pinene	Benzene	353.2	1.40	1.37	-2.1%	1.29	-7.9%	[22]
Alpha-Pinene	Cyclohexane	338.2	1.17	0.95	-18.8%	1.34	14.5%	[22]
Alpha-Pinene	Cyclohexane	353.2	1.08	0.95	-12.0%	1.33	23.1%	[22]
Alpha-Pinene	Ethylbenzene	353.2	1.19	1.29	8.4%	1.28	7.6%	[22]
Alpha-Pinene	Ethylbenzene	373.2	1.17	1.25	6.8%	1.26	7.7%	[22]
Alpha-Pinene	N-Heptane	338.2	1.40	1.29	-7.9%	1.65	17.9%	[22]
Alpha-Pinene	N-Heptane	353.2	1.32	1.27	-3.8%	1.64	24.2%	[22]
Alpha-Pinene	Toluene	353.2	1.21	1.31	8.3%	1.10	-9.1%	[22]
Alpha-Pinene	Toluene	373.2	1.20	1.27	5.8%	1.07	-10.8%	[22]
Aniline	Acetone	277.4	0.59	0.59	0.1%	0.60	1.8%	370
Aniline	Acetone	313.2	0.66	0.70	5.6%	0.79	19.1%	370
Aniline	Acetone	350.8	0.93	0.79	-15.1%	1.02	9.6%	370
Aniline	Acetone	386.7	1.23	0.85	-31.0%	1.19	-3.4%	370
Aniline	Acetonitrile	293.2	1.70	1.17	-31.1%	2.36	39.0%	370
Aniline	Acetonitrile	343.2	1.57	1.12	-28.8%	1.44	-8.4%	370
Aniline	Acetonitrile	393.2	1.58	1.09	-30.9%	1.18	-25.2%	370
Aniline	Chlorobenzene	293.2	3.04	4.33	42.4%	2.57	-15.5%	370
Aniline	Chlorobenzene	343.2	2.22	2.83	27.7%	1.95	-12.0%	370
Aniline	Chlorobenzene	393.2	1.83	2.17	18.9%	1.65	-9.6%	370
Aniline	Ethanol	313.2	3.09	4.29	38.7%	3.28	6.0%	36
Aniline	Ethanol	350.8	2.83	3.57	26.3%	2.75	-2.7%	36
Aniline	Ethanol	386.7	2.44	3.06	25.3%	2.26	-7.5%	36
Aniline	M-Cresol	407.9	0.61	0.75	22.9%	0.66	8.1%	282
Aniline	M-Cresol	407.9	0.66	0.75	13.6%	0.66	0.0%	[61]
Aniline	M-Cresol	408.2	0.66	0.76	15.2%	0.66	0.0%	[61]
Aniline	M-Cresol	422.9	0.65	0.77	19.3%	0.71	10.0%	282
Aniline	M-Cresol	422.9	0.69	0.77	11.6%	0.71	2.9%	[61]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Aniline	M-Cresol	423.2	0.69	0.77	11.6%	0.71	2.9%	[61]
Aniline	M-Cresol	437.9	0.75	0.79	5.0%	0.75	-0.3%	282
Aniline	M-Cresol	437.9	0.74	0.79	6.8%	0.75	1.4%	[61]
Aniline	M-Cresol	438.2	0.74	0.79	6.8%	0.75	1.4%	[61]
Aniline	M-Cresol	453.2	0.74	0.80	7.7%	0.78	5.0%	282
Aniline	M-Cresol	453.2	0.78	0.80	2.6%	0.78	0.0%	[61]
Aniline	N-Methylacetamide	413.5	1.02	0.97	-4.6%	0.77	-24.3%	327
Anisole	1-Butanol	353.2	3.41	2.95	-13.4%	2.46	-27.8%	50
Anisole	1-Octanol	298.2	3.28	2.77	-15.5%	2.42	-26.2%	[3]
Anisole	1-Propanol	358.2	4.49	3.50	-22.0%	2.87	-36.1%	49
Anisole	1-Propanol	368.2	4.12	3.36	-18.4%	2.82	-31.5%	49
Anisole	Alpha-Pinene	353.2	2.28	2.08	-8.8%	1.74	-23.7%	[22]
Anisole	Alpha-Pinene	373.2	1.86	1.93	3.8%	1.55	-16.7%	[22]
Anisole	Benzene	343.2	1.10	1.05	-4.5%	0.95	-13.6%	52
Anisole	Benzene	353.2	1.07	1.05	-1.8%	0.95	-11.2%	52
Anisole	Cyclohexane	343.2	2.45	2.60	6.3%	2.23	-8.8%	53
Anisole	Cyclohexane	353.2	2.44	2.47	1.1%	2.09	-14.5%	53
Anisole	Methyl Ethyl Ketone	333.2	1.66	1.03	-38.0%	1.25	-24.8%	51
Anisole	Methyl Ethyl Ketone	353.2	1.39	1.03	-25.9%	1.41	1.4%	51
Anisole	N-Heptane	358.2	2.28	2.49	9.2%	2.20	-3.5%	55
Anisole	N-Heptane	368.2	2.21	2.38	7.9%	2.10	-4.8%	55
Anisole	N-Hexadecane	298.2	3.19	2.61	-18.3%	2.32	-27.4%	[6]
Anisole	N-Hexane	333.2	2.73	3.01	10.3%	2.68	-1.8%	54
Anisole	N-Hexane	343.2	2.59	2.84	9.7%	2.53	-2.3%	54
Benzene	1,2-Dichloroethane	298.2	1.21	1.08	-10.7%	0.75	-38.0%	121
Benzene	1,2-Dichloroethane	318.4	1.08	1.07	-0.9%	0.75	-30.6%	[12]
Benzene	1,2-Dichloroethane	337.2	1.06	1.07	0.9%	0.75	-29.2%	[12]
Benzene	1,2-Dichloroethane	355.0	1.04	1.06	1.9%	0.75	-27.9%	[12]
Benzene	1,2-Dichloroethane	356.7	1.07	1.06	-0.9%	0.75	-29.9%	[11]
Benzene	1,5-Dimethyl-2-Pyrrolidinone	298.2	0.89	1.01	13.0%	M.G.	N.A.	[29]
Benzene	1,5-Dimethyl-2-Pyrrolidinone	308.2	0.96	1.01	5.6%	M.G.	N.A.	[29]
Benzene	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.02	1.02	0.0%	M.G.	N.A.	[29]
Benzene	1-Butanol	308.2	2.96	2.70	-8.8%	3.14	6.1%	[30]
Benzene	1-Butanol	318.2	2.94	2.64	-10.2%	3.01	2.4%	[30]
Benzene	1-Butanol	328.2	2.81	2.57	-8.5%	2.89	2.8%	[30]
Benzene	1-Ethylpyrrolidin-2-One	298.2	0.86	1.01	16.9%	0.80	-7.4%	[29]
Benzene	1-Ethylpyrrolidin-2-One	308.2	0.98	1.02	4.4%	0.81	-17.1%	[29]
Benzene	1-Ethylpyrrolidin-2-One	318.2	1.09	1.02	-6.4%	0.82	-24.8%	[29]
Benzene	1-Octanol	293.4	1.93	1.82	-5.7%	2.00	3.6%	[31]
Benzene	1-Octanol	298.2	1.99	1.80	-9.5%	1.96	-1.5%	[3]
Benzene	1-Octanol	298.2	2.07	1.80	-13.0%	1.96	-5.3%	[32]
Benzene	1-Octanol	303.5	1.94	1.77	-8.8%	1.91	-1.5%	[31]
Benzene	1-Octanol	313.6	1.83	1.72	-6.0%	1.82	-0.5%	[31]
Benzene	1-Octanol	323.4	1.73	1.67	-3.5%	1.74	0.6%	[31]
Benzene	1-Pentanol	303.5	2.59	2.35	-9.3%	2.70	4.2%	[33]
Benzene	1-Pentanol	308.2	2.93	2.33	-20.5%	2.64	-9.9%	[30]
Benzene	1-Pentanol	313.2	2.59	2.30	-11.2%	2.59	0.0%	[33]
Benzene	1-Pentanol	318.2	2.66	2.28	-14.3%	2.53	-4.9%	[30]
Benzene	1-Pentanol	323.5	2.50	2.25	-10.0%	2.48	-0.8%	[33]
Benzene	1-Pentanol	328.2	2.62	2.22	-15.3%	2.43	-7.3%	[30]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Benzene	1-Phenyl-1-Butanone	298.1	1.03	0.97	-5.8%	0.92	-10.7%	[34]
Benzene	1-Propanol	298.2	3.30	3.49	5.8%	4.12	24.8%	[46]
Benzene	1-Propanol	313.2	3.75	3.37	-10.2%	3.88	3.4%	325
Benzene	2,2,4-Trimethylpentane	313.2	1.57	1.75	11.6%	1.44	-8.2%	277
Benzene	2-Methyl-2-Propanol	313.2	3.16	2.27	-28.2%	3.12	-1.3%	20
Benzene	2-Pyrrolidone	303.2	2.81	3.03	7.9%	M.G.	N.A.	[35]
Benzene	2-Pyrrolidone	313.2	2.83	2.88	1.9%	M.G.	N.A.	[35]
Benzene	2-Pyrrolidone	323.2	2.84	2.75	-3.3%	M.G.	N.A.	[35]
Benzene	2-Pyrrolidone	333.2	2.85	2.63	-7.8%	M.G.	N.A.	[35]
Benzene	Acetone	298.2	1.70	1.62	-4.7%	1.40	-17.6%	[62]
Benzene	Acetone	304.0	1.59	1.60	0.6%	1.39	-12.6%	[12]
Benzene	Acetone	314.4	1.57	1.58	0.6%	1.38	-12.1%	[12]
Benzene	Acetone	323.2	1.50	1.56	4.0%	1.36	-9.3%	268
Benzene	Acetone	329.0	1.54	1.54	0.0%	1.35	-12.3%	[12]
Benzene	Acetone	329.4	1.49	1.54	3.4%	1.35	-9.4%	[11]
Benzene	Acetone	329.4	1.45	1.54	6.2%	1.35	-6.9%	[11]
Benzene	Acetone	333.2	1.60	1.53	-4.4%	1.34	-16.3%	[62]
Benzene	Acetone	373.2	1.50	1.46	-2.7%	1.24	-17.3%	[62]
Benzene	Acetonitrile	293.2	3.19	3.38	6.0%	2.96	-7.2%	[10]
Benzene	Acetonitrile	298.2	2.83	3.26	15.2%	2.92	3.2%	[63]
Benzene	Acetonitrile	298.2	2.90	3.26	12.4%	2.92	0.7%	[64]
Benzene	Acetonitrile	298.2	2.70	3.26	20.7%	2.92	8.1%	[62]
Benzene	Acetonitrile	298.2	3.02	3.26	7.8%	2.92	-3.4%	190
Benzene	Acetonitrile	318.2	2.95	2.88	-2.4%	2.76	-6.4%	[12]
Benzene	Acetonitrile	333.2	2.60	2.65	1.9%	2.65	1.9%	[62]
Benzene	Acetonitrile	348.0	2.60	2.47	-4.8%	2.56	-1.4%	190
Benzene	Acetonitrile	373.2	2.40	2.22	-7.5%	2.43	1.3%	[62]
Benzene	Acetonitrile	397.9	2.31	2.03	-12.2%	2.32	0.4%	190
Benzene	Acetophenone	298.2	1.23	1.24	0.8%	1.22	-0.8%	[65]
Benzene	Alpha-Pinene	353.2	1.18	1.20	1.7%	1.13	-4.2%	[22]
Benzene	Alpha-Pinene	373.2	1.17	1.17	0.0%	1.08	-7.7%	[22]
Benzene	Aniline	293.2	2.22	2.10	-5.4%	1.99	-10.4%	[37]
Benzene	Aniline	293.2	2.24	2.10	-6.3%	1.99	-11.2%	[10]
Benzene	Aniline	298.2	2.20	2.06	-6.4%	1.96	-10.9%	[62]
Benzene	Aniline	298.2	2.34	2.06	-12.0%	1.96	-16.2%	[66]
Benzene	Aniline	298.2	2.24	2.06	-8.0%	1.96	-12.5%	[65]
Benzene	Aniline	333.2	2.00	1.85	-7.5%	1.81	-9.5%	[62]
Benzene	Aniline	373.2	1.80	1.67	-7.2%	1.67	-7.2%	[62]
Benzene	Anisole	293.2	1.05	1.05	0.0%	0.96	-8.6%	[10]
Benzene	Anisole	343.2	1.17	1.03	-11.9%	0.96	-17.9%	52
Benzene	Anisole	353.2	1.12	1.03	-7.8%	0.96	-14.0%	52
Benzene	Benzonitrile	323.2	1.23	1.27	3.6%	M.G.	N.A.	288
Benzene	Benzonitrile	353.2	1.22	1.23	0.8%	M.G.	N.A.	288
Benzene	Benzyl Acetate	298.2	1.04	1.06	1.9%	0.96	-7.7%	[10]
Benzene	Benzyl Alcohol	298.2	2.37	2.00	-15.6%	2.08	-12.2%	[67]
Benzene	Butyl Ether	293.2	0.91	1.02	12.1%	0.99	8.8%	[5]
Benzene	Butyl Ether	308.2	1.00	1.01	0.9%	0.98	-2.1%	135
Benzene	Carbon Tetrachloride	293.2	1.10	1.10	0.0%	1.13	2.7%	[10]
Benzene	Carbon Tetrachloride	313.2	1.13	1.09	-3.1%	1.12	-0.5%	91
Benzene	Carbon Tetrachloride	328.3	1.10	1.09	-0.9%	1.11	0.9%	[12]
Benzene	Carbon Tetrachloride	349.1	1.10	1.08	-1.8%	1.09	-0.9%	[12]
Benzene	Carbon Tetrachloride	349.8	1.10	1.08	-1.8%	1.09	-0.9%	[11]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Benzene	Chloroform	298.7	0.75	0.75	0.0%	0.78	4.0%	[12]
Benzene	Chloroform	319.8	0.83	0.78	-6.0%	0.81	-2.4%	[12]
Benzene	Chloroform	331.9	0.86	0.80	-7.0%	0.82	-4.7%	[12]
Benzene	Chloroform	334.3	0.81	0.80	-1.2%	0.82	1.2%	[11]
Benzene	Chloroform	334.3	0.81	0.80	-1.2%	0.82	1.2%	[11]
Benzene	Cyclohexane	310.9	1.48	1.56	5.4%	1.56	5.4%	[12]
Benzene	Cyclohexane	333.0	1.41	1.48	5.0%	1.45	2.8%	[12]
Benzene	Cyclohexane	352.3	1.35	1.42	5.2%	1.38	2.2%	[12]
Benzene	Cyclohexanone	293.2	0.93	0.99	6.5%	0.98	5.4%	[10]
Benzene	Dichloromethane	298.2	0.92	0.95	3.8%	0.99	8.1%	204
Benzene	Dichloromethane	348.0	0.94	0.96	1.6%	1.00	5.9%	204
Benzene	Diethyl Phthalate	303.2	0.91	0.94	2.8%	M.G.	N.A.	[39]
Benzene	Diethyl Phthalate	313.2	0.92	0.93	1.5%	M.G.	N.A.	[39]
Benzene	Diethyl Phthalate	323.2	0.92	0.92	0.3%	M.G.	N.A.	[39]
Benzene	Diethyl Phthalate	333.2	0.92	0.92	0.2%	M.G.	N.A.	[39]
Benzene	Diisopropyl Ether	343.2	1.13	1.08	-4.8%	1.09	-4.0%	60
Benzene	Dimethyl Carbonate	283.2	1.64	1.29	-21.2%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	293.2	1.60	1.28	-20.1%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	313.2	1.54	1.25	-18.6%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	323.2	1.50	1.24	-17.3%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	333.2	1.47	1.23	-16.2%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	343.2	1.44	1.22	-15.2%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	363.2	1.39	1.21	-12.7%	M.G.	N.A.	239
Benzene	Dimethyl Carbonate	373.2	1.36	1.20	-12.0%	M.G.	N.A.	239
Benzene	Dimethyl Sulfoxide	298.2	3.40	2.41	-29.1%	3.32	-2.4%	[62]
Benzene	Dimethyl Sulfoxide	313.2	3.50	2.26	-35.4%	3.16	-9.7%	[68]
Benzene	Dimethyl Sulfoxide	333.2	3.05	2.09	-31.5%	2.93	-3.9%	[62]
Benzene	Dimethyl Sulfoxide	333.2	3.50	2.09	-40.3%	2.93	-16.3%	[68]
Benzene	Dimethyl Sulfoxide	373.2	2.75	1.85	-32.7%	2.49	-9.5%	[62]
Benzene	Di-N-Propyl Ether	343.2	1.04	0.96	-7.4%	1.02	-1.6%	304
Benzene	Epsilon-Caprolactone	303.2	1.39	1.49	7.2%	M.G.	N.A.	[41]
Benzene	Epsilon-Caprolactone	318.2	1.39	1.45	4.3%	M.G.	N.A.	[41]
Benzene	Epsilon-Caprolactone	333.2	1.41	1.41	0.0%	M.G.	N.A.	[41]
Benzene	Ethanol	296.8	5.40	4.79	-11.3%	5.81	7.6%	[48]
Benzene	Ethanol	298.2	6.00	4.78	-20.3%	5.78	-3.7%	[62]
Benzene	Ethanol	298.2	4.44	4.78	7.7%	5.78	30.2%	[46]
Benzene	Ethanol	298.2	5.21	4.78	-8.3%	5.78	10.9%	[30]
Benzene	Ethanol	313.2	4.26	4.60	8.0%	5.45	27.9%	[46]
Benzene	Ethanol	318.8	5.10	4.53	-11.2%	5.33	4.5%	[48]
Benzene	Ethanol	333.2	5.50	4.31	-21.6%	5.02	-8.7%	[62]
Benzene	Ethanol	334.7	4.70	4.29	-8.7%	4.99	6.2%	[48]
Benzene	Ethanol	346.4	4.40	4.11	-6.6%	4.76	8.2%	[12]
Benzene	Ethanol	353.2	4.40	4.00	-9.1%	4.62	5.0%	[48]
Benzene	Ethanol	373.2	5.00	3.69	-26.2%	4.27	-14.6%	[62]
Benzene	Ethyl Acetate	311.7	1.14	1.16	1.8%	1.12	-1.8%	[12]
Benzene	Ethyl Acetate	328.2	0.96	1.15	19.5%	1.10	14.3%	229
Benzene	Ethyl Acetate	330.5	1.14	1.15	0.9%	1.09	-4.4%	[12]
Benzene	Ethyl Benzoate	313.2	0.96	0.94	-1.6%	M.G.	N.A.	[41]
Benzene	Ethyl Benzoate	323.2	0.96	0.94	-2.0%	M.G.	N.A.	[41]
Benzene	Ethyl Benzoate	333.2	0.96	0.94	-2.4%	M.G.	N.A.	[41]
Benzene	Ethyl Benzoate	343.2	0.97	0.94	-2.8%	M.G.	N.A.	[41]
Benzene	Glutaronitrile	303.2	3.51	3.66	4.3%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Benzene	Glutaronitrile	313.2	3.42	3.42	0.0%	M.G.	N.A.	[39]
Benzene	Glutaronitrile	323.2	3.37	3.21	-4.7%	M.G.	N.A.	[39]
Benzene	Glutaronitrile	333.2	3.30	3.03	-8.2%	M.G.	N.A.	[39]
Benzene	Isopropanol	298.2	4.24	3.56	-16.0%	3.96	-6.6%	[63]
Benzene	Isopropanol	298.2	4.50	3.56	-20.9%	3.96	-12.0%	[64]
Benzene	Isopropanol	313.2	3.68	3.43	-6.8%	3.73	1.3%	325
Benzene	Methanol	298.2	6.82	7.44	9.1%	7.22	5.9%	[63]
Benzene	Methanol	298.2	7.00	7.44	6.3%	7.22	3.1%	[64]
Benzene	Methanol	298.2	7.50	7.44	-0.8%	7.22	-3.7%	[62]
Benzene	Methanol	298.2	6.47	7.44	15.0%	7.22	11.6%	[46]
Benzene	Methanol	298.2	7.17	7.44	3.8%	7.22	0.7%	[30]
Benzene	Methanol	303.2	7.17	7.33	2.2%	7.14	-0.4%	[69]
Benzene	Methanol	333.2	5.80	6.46	11.4%	6.65	14.7%	[62]
Benzene	Methanol	373.2	4.70	5.17	10.0%	5.90	25.5%	[62]
Benzene	Methyl Ethyl Ketone	298.2	1.12	1.17	4.5%	1.20	7.1%	[62]
Benzene	Methyl Ethyl Ketone	333.2	1.15	1.16	0.9%	1.18	2.6%	[11]
Benzene	Methyl Ethyl Ketone	352.8	1.22	1.15	-5.7%	1.16	-4.9%	[62]
Benzene	Methyl Ethyl Ketone	373.2	1.30	1.15	-11.5%	1.12	-13.8%	[62]
Benzene	Methyl Isobutyl Ketone	293.2	0.87	0.97	11.5%	0.99	13.8%	[5]
Benzene	Methyl Isobutyl Ketone	348.2	1.09	0.98	-10.1%	0.99	-9.2%	[49]
Benzene	N,N-Dibutylformamide	302.8	0.82	0.77	-6.3%	0.79	-3.9%	[13]
Benzene	N,N-Dibutylformamide	318.3	0.84	0.78	-7.6%	0.79	-6.4%	[13]
Benzene	N,N-Dibutylformamide	332.4	0.86	0.79	-8.2%	0.79	-8.2%	[13]
Benzene	N,N-Diethylacetamide	303.2	0.95	0.99	4.4%	0.94	-0.8%	[39]
Benzene	N,N-Diethylacetamide	313.2	0.97	0.99	2.0%	0.94	-3.2%	[39]
Benzene	N,N-Diethylacetamide	323.2	0.99	0.99	0.0%	0.94	-5.1%	[39]
Benzene	N,N-Diethylacetamide	333.2	1.01	0.99	-2.0%	0.94	-6.9%	[39]
Benzene	N,N-Dimethylacetamide	303.6	1.14	1.24	8.5%	1.05	-8.1%	[13]
Benzene	N,N-Dimethylacetamide	317.6	1.17	1.23	5.5%	1.06	-9.1%	[13]
Benzene	N,N-Dimethylacetamide	333.6	1.19	1.22	2.6%	1.07	-10.0%	[13]
Benzene	N,N-Dimethylformamide	298.2	1.40	1.86	32.9%	1.70	21.4%	[62]
Benzene	N,N-Dimethylformamide	298.2	1.43	1.86	30.1%	1.70	18.9%	[65]
Benzene	N,N-Dimethylformamide	333.2	1.40	1.68	20.0%	1.69	20.7%	[62]
Benzene	N,N-Dimethylformamide	373.2	1.35	1.54	14.1%	1.68	24.4%	[62]
Benzene	N-Ethylacetamide	303.2	2.43	2.21	-9.1%	M.G.	N.A.	[39]
Benzene	N-Ethylacetamide	313.2	2.42	2.17	-10.3%	M.G.	N.A.	[39]
Benzene	N-Ethylacetamide	323.2	2.44	2.14	-12.3%	M.G.	N.A.	[39]
Benzene	N-Ethylacetamide	333.2	2.43	2.10	-13.6%	M.G.	N.A.	[39]
Benzene	N-Formylmorpholine	313.3	2.05	2.51	22.4%	M.G.	N.A.	[43]
Benzene	N-Formylmorpholine	332.7	1.96	2.31	17.9%	M.G.	N.A.	[43]
Benzene	N-Formylmorpholine	352.5	1.94	2.14	10.3%	M.G.	N.A.	[43]
Benzene	N-Formylmorpholine	373.4	1.86	2.00	7.5%	M.G.	N.A.	[43]
Benzene	N-Heptane	298.2	1.55	1.64	5.8%	1.62	4.5%	[62]
Benzene	N-Heptane	313.2	1.52	1.56	2.4%	1.53	0.4%	104
Benzene	N-Heptane	331.2	1.37	1.48	8.0%	1.44	5.1%	[12]
Benzene	N-Heptane	333.2	1.38	1.48	7.1%	1.43	3.5%	104
Benzene	N-Heptane	333.2	1.40	1.48	5.7%	1.43	2.1%	[62]
Benzene	N-Heptane	350.6	1.33	1.42	6.8%	1.36	2.3%	[12]
Benzene	N-Heptane	366.2	1.27	1.37	7.9%	1.30	2.4%	[12]
Benzene	N-Heptane	373.2	1.22	1.35	10.7%	1.28	4.9%	[62]
Benzene	N-Hexadecane	293.2	1.09	1.11	1.8%	1.10	0.9%	[70]
Benzene	N-Hexadecane	298.2	1.06	1.09	2.8%	1.07	0.9%	[70]

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Benzene	N-Hexadecane	298.2	1.06	1.09	3.0%	1.07	1.1%	[6]
Benzene	N-Hexadecane	303.2	1.04	1.07	2.9%	1.05	1.0%	[70]
Benzene	N-Hexadecane	313.2	1.00	1.04	4.0%	1.01	1.0%	[70]
Benzene	N-Hexadecane	323.2	0.98	1.01	3.1%	0.98	0.0%	[70]
Benzene	N-Hexadecane	333.2	0.96	0.99	3.1%	0.95	-1.0%	[70]
Benzene	N-Hexadecane	333.2	0.89	0.99	11.2%	0.95	6.7%	[71]
Benzene	N-Hexadecane	393.2	0.80	0.88	10.0%	0.81	1.3%	[71]
Benzene	N-Hexadecane	453.2	0.74	0.82	10.8%	0.72	-2.7%	[71]
Benzene	N-Hexane	313.2	1.60	1.67	4.3%	1.65	3.0%	105
Benzene	N-Hexane	342.0	1.41	1.54	9.2%	1.50	6.4%	[11]
Benzene	Nitrobenzene	293.2	1.39	1.35	-2.9%	1.30	-6.5%	[10]
Benzene	Nitrobenzene	298.2	1.20	1.34	11.7%	1.30	8.3%	[62]
Benzene	Nitrobenzene	298.2	1.41	1.34	-5.0%	1.30	-7.8%	[65]
Benzene	Nitrobenzene	333.2	1.10	1.28	16.4%	1.27	15.5%	[62]
Benzene	Nitrobenzene	373.2	1.00	1.23	23.0%	1.23	23.0%	[62]
Benzene	Nitroethane	293.2	1.82	1.98	8.8%	1.73	-4.9%	[10]
Benzene	Nitromethane	293.2	3.86	3.84	-0.5%	3.80	-1.6%	[10]
Benzene	Nitromethane	298.2	3.20	3.69	15.3%	3.72	16.3%	[62]
Benzene	Nitromethane	333.2	2.90	2.94	1.4%	3.11	7.2%	[62]
Benzene	Nitromethane	358.9	3.06	2.58	-15.7%	2.67	-12.7%	[12]
Benzene	Nitromethane	371.5	2.65	2.44	-7.9%	2.46	-7.2%	[12]
Benzene	Nitromethane	373.2	2.60	2.42	-6.9%	2.43	-6.5%	[62]
Benzene	N-Methyl-2-Pyrrolidone	323.4	1.27	1.17	-7.9%	0.98	-22.8%	[43]
Benzene	N-Methyl-2-Pyrrolidone	333.2	1.23	1.17	-4.9%	1.00	-18.7%	[43]
Benzene	N-Methyl-2-Pyrrolidone	333.3	0.74	1.17	57.1%	1.00	34.3%	41
Benzene	N-Methyl-2-Pyrrolidone	343.4	1.28	1.17	-8.6%	1.02	-20.3%	[43]
Benzene	N-Methyl-2-Pyrrolidone	354.2	0.83	1.17	40.2%	1.05	25.8%	41
Benzene	N-Methylacetamide	303.3	3.52	2.85	-19.1%	2.88	-18.2%	[13]
Benzene	N-Methylacetamide	318.4	3.34	2.77	-16.9%	2.84	-14.8%	[13]
Benzene	N-Methylacetamide	333.3	2.98	2.67	-10.5%	2.80	-6.2%	[13]
Benzene	N-Methylformamide	303.2	5.01	4.83	-3.7%	M.P.	N.A.	[35]
Benzene	N-Methylformamide	313.2	4.92	4.63	-5.8%	M.P.	N.A.	[35]
Benzene	N-Methylformamide	323.2	4.84	4.43	-8.4%	M.P.	N.A.	[35]
Benzene	N-Methylformamide	333.2	4.75	4.23	-11.0%	M.P.	N.A.	[35]
Benzene	N-Nonane	313.2	0.97	1.39	43.3%	1.36	40.2%	[72]
Benzene	N-Nonane	323.2	0.96	1.35	40.6%	1.31	36.5%	[72]
Benzene	N-Nonane	333.2	0.96	1.32	37.5%	1.27	32.3%	[72]
Benzene	Phenol	298.2	2.90	2.25	-22.4%	2.22	-23.4%	[62]
Benzene	Phenol	328.2	2.87	2.16	-24.7%	2.05	-28.6%	[14]
Benzene	Phenol	333.2	2.50	2.15	-14.0%	2.02	-19.2%	[62]
Benzene	Phenol	343.2	2.62	2.11	-19.5%	1.96	-25.2%	[14]
Benzene	Phenol	353.2	2.11	2.07	-1.8%	1.91	-9.4%	582
Benzene	Phenol	358.2	2.53	2.05	-19.0%	1.88	-25.7%	[14]
Benzene	Phenol	373.2	2.20	1.99	-9.5%	1.80	-18.2%	[62]
Benzene	Phenol	373.2	2.49	1.99	-20.1%	1.80	-27.7%	[14]
Benzene	Propionitrile	293.2	1.84	1.88	2.2%	1.76	-4.3%	[10]
Benzene	Propionitrile	298.2	1.58	1.85	17.1%	1.76	11.4%	[62]
Benzene	Propionitrile	333.2	1.48	1.67	12.8%	1.74	17.6%	[62]
Benzene	Propionitrile	373.2	1.40	1.54	10.0%	1.72	22.9%	[62]
Benzene	P-Xylene	293.2	0.99	1.02	3.0%	1.02	3.0%	[10]
Benzene	P-Xylene	308.2	1.05	1.01	-3.8%	1.01	-3.8%	133
Benzene	P-Xylene	313.2	0.88	1.01	14.8%	1.01	14.8%	[72]

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Benzene	P-Xylene	323.2	0.85	1.01	18.8%	1.00	17.6%	[72]
Benzene	P-Xylene	333.2	0.98	1.01	3.1%	0.99	1.0%	[72]
Benzene	Pyridine	298.2	1.20	1.37	14.4%	1.13	-5.6%	82
Benzene	Pyridine	298.2	1.20	1.37	14.2%	1.13	-5.8%	[62]
Benzene	Pyridine	303.2	1.20	1.36	13.6%	1.13	-5.6%	82
Benzene	Pyridine	313.2	1.20	1.34	11.4%	1.13	-6.1%	82
Benzene	Pyridine	323.2	1.18	1.32	12.0%	1.13	-4.2%	82
Benzene	Pyridine	333.2	1.20	1.30	8.3%	1.13	-5.8%	[62]
Benzene	Pyridine	373.2	1.20	1.24	3.3%	1.16	-3.3%	[62]
Benzene	Quinoline	293.2	1.67	1.39	-16.8%	M.G.	N.A.	[37]
Benzene	Quinoline	298.2	1.32	1.38	4.5%	M.G.	N.A.	[10]
Benzene	Sulfolane	303.8	2.38	2.69	13.1%	M.G.	N.A.	[13]
Benzene	Sulfolane	317.9	2.35	2.49	6.1%	M.G.	N.A.	[13]
Benzene	Sulfolane	333.7	2.32	2.31	-0.2%	M.G.	N.A.	[13]
Benzene	Tetraethylene Glycol DME	303.2	0.69	0.75	8.1%	0.61	-12.1%	[7]
Benzene	Tetraethylene Glycol DME	323.2	0.71	0.76	6.7%	0.62	-12.9%	[7]
Benzene	Tetraethylene Glycol DME	343.5	0.74	0.76	2.6%	0.62	-16.3%	[7]
Benzene	Toluene	293.2	0.99	1.00	1.0%	1.01	2.0%	[10]
Benzene	Toluene	298.2	0.98	1.00	2.0%	1.01	3.1%	[69]
Benzene	Tributyl Phosphate	298.2	0.69	0.53	-23.2%	M.G.	N.A.	[20]
Benzene	Tributyl Phosphate	298.6	0.62	0.53	-14.5%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	302.9	0.63	0.54	-14.3%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	308.6	0.63	0.54	-14.3%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	313.1	0.64	0.54	-15.6%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	318.2	0.66	0.55	-16.7%	M.G.	N.A.	[20]
Benzene	Tributyl Phosphate	323.7	0.63	0.55	-12.7%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	330.0	0.60	0.55	-8.3%	M.G.	N.A.	[27]
Benzene	Tributyl Phosphate	333.2	0.66	0.55	-16.7%	M.G.	N.A.	[20]
Benzene	Tributyl Phosphate	333.2	0.62	0.55	-11.3%	M.G.	N.A.	[73]
Benzene	Tributyl Phosphate	363.2	0.65	0.56	-13.8%	M.G.	N.A.	[20]
Benzene	Tributyl Phosphate	373.2	0.65	0.57	-12.3%	M.G.	N.A.	[20]
Benzene	Triethylamine	323.5	1.28	1.23	-3.9%	1.13	-11.7%	[12]
Benzene	Triethylamine	348.7	1.22	1.20	-1.6%	1.10	-9.8%	[12]
Benzene	Triethylamine	359.3	1.08	1.19	10.2%	1.08	0.0%	[12]
Benzonitrile	1-Octanol	298.2	6.86	4.63	-32.5%	M.G.	N.A.	[3]
Benzonitrile	Benzene	323.2	1.51	1.44	-4.9%	M.G.	N.A.	288
Benzonitrile	Benzene	353.2	1.49	1.38	-7.6%	M.G.	N.A.	288
Benzonitrile	N-Hexadecane	298.2	16.95	7.68	-54.7%	M.G.	N.A.	[6]
Benzonitrile	Toluene	323.2	1.69	1.71	1.1%	M.G.	N.A.	288
Benzonitrile	Toluene	353.2	1.65	1.59	-3.5%	M.G.	N.A.	288
Benzyl Alcohol	Acetophenone	413.2	1.03	0.96	-6.6%	0.94	-8.5%	324
Benzyl Alcohol	Acetophenone	473.2	1.03	0.97	-6.0%	0.66	-36.1%	324
Bromoethane	1,2-Dichloroethane	293.2	1.18	1.11	-5.9%	1.23	4.2%	[10]
Bromoethane	1-Butanol	293.2	2.66	2.51	-5.6%	2.75	3.4%	[10]
Bromoethane	1-Chlorobutane	293.2	1.02	0.99	-2.9%	0.90	-11.8%	[10]
Bromoethane	1-Octanol	293.2	1.99	1.71	-14.1%	1.91	-4.0%	[10]
Bromoethane	2,2,4-Trimethylpentane	293.2	1.63	1.63	0.0%	1.50	-8.0%	[10]
Bromoethane	2-Nitropropane	293.2	1.53	1.34	-12.4%	1.72	12.4%	[10]
Bromoethane	Acetonitrile	293.2	2.88	2.85	-1.0%	3.34	16.0%	[10]
Bromoethane	Acetophenone	293.2	1.18	1.20	1.7%	1.77	50.0%	[10]
Bromoethane	Aniline	293.2	2.14	2.03	-5.1%	M.P.	N.A.	[10]
Bromoethane	Anisole	293.2	1.08	1.03	-4.6%	M.P.	N.A.	[10]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Bromoethane	Benzene	293.2	1.01	1.03	2.0%	1.25	23.8%	[58]
Bromoethane	Benzene	293.2	1.01	1.03	2.0%	1.25	23.8%	[10]
Bromoethane	Benzonitrile	293.2	1.33	1.21	-9.0%	M.G.	N.A.	[10]
Bromoethane	Benzyl Acetate	298.2	1.02	1.00	-2.0%	1.28	25.5%	[10]
Bromoethane	Carbon Tetrachloride	293.2	1.25	1.19	-4.8%	1.40	12.0%	[10]
Bromoethane	Chloroform	305.0	0.82	0.82	0.0%	M.P.	N.A.	[12]
Bromoethane	Chloroform	323.0	0.83	0.84	1.2%	M.P.	N.A.	[12]
Bromoethane	Cyclohexanone	293.2	0.96	1.00	4.2%	1.07	11.5%	[10]
Bromoethane	Ethanol	293.2	4.19	4.10	-2.1%	4.06	-3.1%	[10]
Bromoethane	Ethyl Acetate	293.2	1.04	1.03	-1.0%	1.12	7.7%	[10]
Bromoethane	Methyl Ethyl Ketone	293.2	1.14	1.08	-5.3%	1.11	-2.6%	[10]
Bromoethane	Methyl Ethyl Ketone	314.7	1.05	1.07	1.9%	1.14	8.6%	[12]
Bromoethane	Methyl Ethyl Ketone	333.3	1.00	1.07	7.0%	1.14	14.0%	[12]
Bromoethane	N,N-Dimethylformamide	293.2	1.65	1.92	16.4%	M.P.	N.A.	[10]
Bromoethane	N-Heptane	293.2	1.62	1.60	-1.2%	1.55	-4.3%	[10]
Bromoethane	N-Hexane	301.0	1.62	1.64	1.2%	1.55	-4.3%	[12]
Bromoethane	N-Hexane	314.3	1.54	1.57	1.9%	1.46	-5.2%	[12]
Bromoethane	N-Hexane	332.0	1.37	1.49	8.8%	1.35	-1.5%	[12]
Bromoethane	N-Hexane	340.3	1.26	1.45	15.1%	1.31	4.0%	[12]
Bromoethane	Nitrobenzene	293.2	1.50	1.26	-16.0%	1.50	0.0%	[10]
Bromoethane	Nitroethane	293.2	1.70	1.73	1.8%	2.25	32.4%	[10]
Bromoethane	Nitromethane	293.2	3.56	3.17	-11.0%	6.63	86.2%	[10]
Bromoethane	N-Octane	293.2	1.69	1.52	-10.2%	1.50	-11.3%	[10]
Bromoethane	Phenol	323.2	2.05	2.27	10.7%	M.P.	N.A.	[10]
Bromoethane	Propionitrile	293.2	1.73	1.71	-1.2%	1.78	2.9%	[10]
Bromoethane	P-Xylene	293.2	1.00	0.99	-1.0%	0.89	-11.0%	[10]
Bromoethane	Quinoline	298.2	1.27	1.39	9.4%	M.G.	N.A.	[10]
Bromoethane	Toluene	293.2	0.98	1.02	4.1%	1.02	4.1%	[10]
Bromoethane	Triethylamine	348.7	1.02	1.15	12.7%	M.P.	N.A.	[12]
Butanal	1-Hexene	298.2	2.76	2.70	-2.2%	2.22	-19.7%	[38]
Butanal	1-Hexene	318.2	2.36	2.41	2.1%	2.04	-13.6%	[38]
Butanal	1-Hexene	336.2	2.21	2.21	0.0%	1.91	-13.4%	[38]
Butanal	1-Pentanol	303.5	2.87	2.71	-5.6%	0.46	-84.0%	[33]
Butanal	1-Pentanol	313.2	2.62	2.61	-0.4%	0.70	-73.5%	[33]
Butanal	1-Pentanol	323.5	2.42	2.52	4.1%	0.91	-62.4%	[33]
Butanal	Acetone	328.2	1.07	1.15	7.5%	1.02	-4.3%	[49]
Butanal	Ethyl Acetate	298.2	1.11	1.01	-9.0%	1.16	4.1%	[49]
Butanal	Ethyl Acetate	323.2	1.10	1.01	-8.2%	1.10	0.1%	[49]
Butanal	Ethyl Acetate	349.2	1.09	1.01	-7.3%	1.06	-2.9%	[38]
Butanal	Hexadecane	298.2	2.60	2.56	-1.6%	2.71	4.0%	[38]
Butanal	Methyl Isobutyl Ketone	328.2	1.10	1.00	-9.1%	1.03	-6.2%	[38]
Butanal	Methyl Isobutyl Ketone	348.2	1.07	1.00	-6.5%	1.01	-5.7%	[38]
Butanal	Methyl Isobutyl Ketone	388.2	1.03	0.99	-3.9%	0.97	-5.7%	[6]
Butanal	N-Formylmorpholine	303.5	2.09	2.23	6.7%	M.G.	N.A.	[43]
Butanal	N-Formylmorpholine	323.2	2.01	2.08	3.5%	M.G.	N.A.	[43]
Butanal	N-Formylmorpholine	342.8	1.96	1.95	-0.5%	M.G.	N.A.	[43]
Butanal	N-Hexane	303.2	3.46	3.31	-4.3%	3.71	7.1%	[38]
Butanal	N-Hexane	323.2	3.12	2.89	-7.4%	3.29	5.6%	[38]
Butanal	N-Hexane	341.2	2.84	2.61	-8.1%	3.01	5.8%	[38]
Butanal	N-Methylpyrrolidone	323.4	1.51	1.49	-1.3%	M.P.	N.A.	[43]
Butanal	N-Methylpyrrolidone	333.2	1.48	1.46	-1.4%	M.P.	N.A.	[43]
Butanal	N-Methylpyrrolidone	343.4	1.51	1.44	-4.6%	M.P.	N.A.	[43]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Butanal	Tetrahydrofuran	293.7	1.21	1.09	-9.9%	M.P.	N.A.	[12]
Butanal	Tetrahydrofuran	311.5	1.13	1.08	-4.4%	M.P.	N.A.	[12]
Butanal	Tetrahydrofuran	328.4	1.10	1.08	-1.8%	M.P.	N.A.	[12]
Butanal	Tetrahydrofuran	336.9	1.09	1.07	-1.8%	M.P.	N.A.	[12]
Butyl Acetate	1-Octanol	298.2	2.11	1.97	-6.6%	2.04	-3.3%	[3]
Butyl Acetate	N,N-Dibutylformamide	302.8	1.29	1.10	-14.8%	1.08	-16.3%	[13]
Butyl Acetate	N,N-Dibutylformamide	318.3	1.27	1.09	-14.2%	1.09	-14.2%	[13]
Butyl Acetate	N,N-Dibutylformamide	332.5	1.25	1.08	-13.7%	1.11	-11.3%	[13]
Butyl Acetate	N,N-Dimethylacetamide	303.3	2.37	1.99	-15.9%	0.83	-64.9%	[13]
Butyl Acetate	N,N-Dimethylacetamide	317.6	2.03	1.89	-6.9%	0.83	-59.1%	[13]
Butyl Acetate	N,N-Dimethylacetamide	333.2	1.74	1.79	2.8%	0.84	-51.8%	[13]
Butyl Acetate	N-Hexadecane	298.2	2.22	2.11	-4.7%	3.13	41.3%	[6]
Butyl Acetate	N-Methylacetamide	303.0	3.55	3.78	6.5%	2.85	-19.7%	[13]
Butyl Acetate	N-Methylacetamide	318.4	3.55	3.61	1.7%	2.74	-22.8%	[13]
Butyl Acetate	N-Methylacetamide	333.2	3.46	3.44	-0.5%	2.65	-23.3%	[13]
Butyl Acetate	Sulfolane	303.1	4.99	5.78	15.9%	M.G.	N.A.	[13]
Butyl Acetate	Sulfolane	317.9	4.67	5.01	7.3%	M.G.	N.A.	[13]
Butyl Acetate	Sulfolane	334.2	4.45	4.36	-2.1%	M.G.	N.A.	[13]
Butyl Acetate	Tetraethylene Glycol DME	303.2	1.05	1.17	11.3%	0.79	-24.8%	[7]
Butyl Acetate	Tetraethylene Glycol DME	323.2	1.04	1.14	10.1%	0.89	-14.0%	[7]
Butyl Acetate	Tetraethylene Glycol DME	343.2	1.01	1.12	10.5%	1.05	3.6%	[7]
Butyl Acetate	Tributyl Phosphate	298.6	0.98	0.76	-22.4%	M.G.	N.A.	[27]
Butyl Acetate	Tributyl Phosphate	302.9	0.98	0.76	-22.4%	M.G.	N.A.	[27]
Butyl Acetate	Tributyl Phosphate	308.6	0.98	0.76	-22.4%	M.G.	N.A.	[27]
Butyl Acetate	Tributyl Phosphate	313.1	0.99	0.76	-23.2%	M.G.	N.A.	[27]
Butyl Ether	1-Octanol	298.2	2.27	1.73	-23.8%	2.01	-11.5%	[3]
Butyl Ether	Benzene	308.2	1.10	1.06	-3.3%	1.16	5.8%	135
Butyl Ether	Carbon Tetrachloride	308.2	0.79	0.68	-13.4%	0.82	4.4%	134
Butyl Ether	N-Hexadecane	298.2	1.20	1.18	-1.9%	1.06	-11.9%	[6]
Butyl Ether	N-Hexane	308.2	1.09	1.18	8.5%	1.11	2.1%	136
Butyronitrile	1-Butanol	278.2	5.29	4.49	-15.1%	1.40	-73.5%	27
Butyronitrile	1-Butanol	288.2	4.29	4.21	-1.8%	1.44	-66.4%	27
Butyronitrile	1-Butanol	293.2	4.10	4.08	-0.4%	1.45	-64.6%	27
Butyronitrile	1-Butanol	298.2	3.96	3.96	0.0%	1.44	-63.6%	27
Butyronitrile	1-Butanol	303.2	3.80	3.85	1.3%	1.43	-62.4%	27
Butyronitrile	1-Butanol	308.2	3.56	3.74	5.2%	1.42	-60.1%	27
Butyronitrile	1-Butanol	313.2	3.44	3.63	5.5%	1.39	-59.6%	27
Butyronitrile	1-Butanol	323.2	3.20	3.44	7.7%	1.33	-58.4%	27
Butyronitrile	1-Octanol	288.2	5.35	4.86	-9.2%	1.46	-72.7%	23
Butyronitrile	1-Octanol	293.2	4.67	4.64	-0.6%	1.46	-68.7%	23
Butyronitrile	1-Octanol	298.2	4.80	4.44	-7.6%	1.45	-69.8%	23
Butyronitrile	1-Octanol	298.2	4.72	4.44	-5.9%	1.45	-69.3%	[3]
Butyronitrile	1-Octanol	303.2	4.08	4.25	4.2%	1.43	-64.9%	23
Butyronitrile	1-Octanol	308.2	3.85	4.08	5.9%	1.41	-63.4%	23
Butyronitrile	1-Octanol	313.2	3.72	3.92	5.3%	1.38	-62.9%	23
Butyronitrile	1-Octanol	323.2	3.27	3.64	11.2%	1.31	-60.0%	23
Butyronitrile	1-Propanol	278.2	6.69	4.95	-26.0%	1.41	-78.9%	29
Butyronitrile	1-Propanol	288.2	4.82	4.64	-3.8%	1.45	-69.9%	29
Butyronitrile	1-Propanol	293.2	4.50	4.49	-0.2%	1.46	-67.6%	29
Butyronitrile	1-Propanol	298.2	4.09	4.35	6.5%	1.46	-64.3%	29
Butyronitrile	1-Propanol	303.2	3.94	4.22	7.0%	1.46	-63.0%	29
Butyronitrile	1-Propanol	308.2	3.71	4.10	10.4%	1.44	-61.2%	29

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Butyronitrile	1-Propanol	313.2	3.52	3.98	13.0%	1.42	-59.7%	29
Butyronitrile	1-Propanol	323.2	3.18	3.77	18.7%	1.36	-57.2%	29
Butyronitrile	2-Butanol	278.2	7.69	4.93	-35.9%	1.40	-81.8%	26
Butyronitrile	2-Butanol	288.2	5.83	4.58	-21.4%	1.44	-75.3%	26
Butyronitrile	2-Butanol	293.2	4.75	4.42	-6.9%	1.45	-69.4%	26
Butyronitrile	2-Butanol	298.2	4.59	4.27	-7.0%	1.44	-68.6%	26
Butyronitrile	2-Butanol	303.2	3.90	4.13	5.9%	1.43	-63.3%	26
Butyronitrile	2-Butanol	308.2	3.71	3.99	7.6%	1.42	-61.7%	26
Butyronitrile	2-Butanol	313.2	3.30	3.87	17.4%	1.39	-57.8%	26
Butyronitrile	2-Butanol	323.2	2.90	3.64	25.5%	1.33	-54.2%	26
Butyronitrile	2-Methyl-1-Propanol	278.2	6.13	4.47	-27.1%	1.40	-77.2%	25
Butyronitrile	2-Methyl-1-Propanol	288.2	5.04	4.18	-17.0%	1.44	-71.4%	25
Butyronitrile	2-Methyl-1-Propanol	293.2	4.96	4.05	-18.4%	1.45	-70.8%	25
Butyronitrile	2-Methyl-1-Propanol	298.2	4.43	3.92	-11.5%	1.44	-67.5%	25
Butyronitrile	2-Methyl-1-Propanol	303.2	4.12	3.81	-7.6%	1.43	-65.3%	25
Butyronitrile	2-Methyl-1-Propanol	308.2	3.83	3.69	-3.8%	1.42	-63.0%	25
Butyronitrile	2-Methyl-1-Propanol	313.2	3.51	3.59	2.2%	1.39	-60.4%	25
Butyronitrile	2-Methyl-1-Propanol	323.2	3.09	3.40	10.1%	1.33	-56.9%	25
Butyronitrile	2-Methyl-2-Propanol	298.2	3.69	3.26	-11.6%	1.25	-66.1%	24
Butyronitrile	2-Methyl-2-Propanol	303.2	3.33	3.18	-4.6%	1.24	-62.8%	24
Butyronitrile	2-Methyl-2-Propanol	308.2	3.05	3.10	1.6%	1.22	-60.0%	24
Butyronitrile	2-Methyl-2-Propanol	313.2	2.88	3.03	5.2%	1.20	-58.3%	24
Butyronitrile	2-Methyl-2-Propanol	318.2	2.78	2.95	6.2%	1.18	-57.5%	24
Butyronitrile	2-Methyl-2-Propanol	323.2	2.62	2.89	10.5%	1.15	-56.0%	24
Butyronitrile	Ethanol	278.2	4.53	4.22	-6.8%	1.46	-67.8%	30
Butyronitrile	Ethanol	288.2	4.16	4.06	-2.5%	1.51	-63.7%	30
Butyronitrile	Ethanol	293.2	3.95	3.98	0.9%	1.53	-61.2%	30
Butyronitrile	Ethanol	298.2	3.86	3.90	1.0%	1.53	-60.4%	30
Butyronitrile	Ethanol	303.2	3.70	3.82	3.3%	1.52	-58.9%	30
Butyronitrile	Ethanol	308.2	3.63	3.75	3.3%	1.51	-58.4%	30
Butyronitrile	Ethanol	313.2	3.50	3.67	4.8%	1.49	-57.4%	30
Butyronitrile	Ethanol	323.2	3.37	3.52	4.6%	1.42	-57.8%	30
Butyronitrile	Isopropanol	278.2	4.67	4.72	1.2%	1.30	-72.1%	28
Butyronitrile	Isopropanol	288.2	4.33	4.45	2.8%	1.34	-69.0%	28
Butyronitrile	Isopropanol	293.2	4.10	4.32	5.4%	1.35	-67.1%	28
Butyronitrile	Isopropanol	298.2	3.92	4.20	7.0%	1.35	-65.6%	28
Butyronitrile	Isopropanol	303.2	3.82	4.08	6.8%	1.34	-64.9%	28
Butyronitrile	Isopropanol	308.2	3.64	3.97	9.1%	1.33	-63.5%	28
Butyronitrile	Isopropanol	313.2	3.55	3.87	9.1%	1.31	-63.1%	28
Butyronitrile	Isopropanol	323.2	3.15	3.67	16.6%	1.25	-60.3%	28
Butyronitrile	Methanol	278.2	3.97	3.60	-9.3%	0.92	-76.8%	31
Butyronitrile	Methanol	288.2	3.56	3.52	-1.2%	0.95	-73.3%	31
Butyronitrile	Methanol	298.2	3.45	3.44	-0.2%	0.96	-72.1%	31
Butyronitrile	Methanol	308.2	3.31	3.34	1.0%	0.97	-70.7%	31
Butyronitrile	Methanol	318.2	3.17	3.23	1.8%	0.96	-69.8%	31
Butyronitrile	N-Hexadecane	298.2	11.63	8.19	-29.6%	6.89	-40.8%	[6]
Butyronitrile	Tributyl Phosphate	302.9	0.83	0.89	7.2%	M.G.	N.A.	[27]
Butyronitrile	Tributyl Phosphate	308.6	0.83	0.88	6.0%	M.G.	N.A.	[27]
Butyronitrile	Tributyl Phosphate	313.1	0.85	0.87	2.4%	M.G.	N.A.	[27]
Butyronitrile	Tributyl Phosphate	323.7	0.79	0.86	8.9%	M.G.	N.A.	[27]
Carbon Disulfide	1,2-Dichloroethane	293.2	2.58	2.03	-21.3%	M.P.	N.A.	[10]
Carbon Disulfide	1-Butanol	293.2	3.14	3.26	3.8%	M.P.	N.A.	[10]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Carbon Disulfide	1-Chlorobutane	293.2	1.56	1.54	-1.3%	1.63	4.5%	[10]
Carbon Disulfide	1-Octanol	293.2	1.75	1.80	2.9%	M.P.	N.A.	[10]
Carbon Disulfide	2,2,4-Trimethylpentane	293.2	1.33	1.60	20.3%	1.27	-4.5%	[10]
Carbon Disulfide	2-Nitropropane	293.2	4.03	3.60	-10.7%	3.36	-16.6%	[10]
Carbon Disulfide	Acetone	300.9	4.22	4.19	-0.7%	4.15	-1.7%	[17]
Carbon Disulfide	Acetone	306.9	4.09	4.05	-1.0%	4.04	-1.2%	[17]
Carbon Disulfide	Acetone	313.9	3.88	3.91	0.8%	3.93	1.3%	[17]
Carbon Disulfide	Acetone	319.5	3.78	3.80	0.5%	3.84	1.6%	[17]
Carbon Disulfide	Acetone	324.4	3.65	3.71	1.6%	3.76	3.0%	[17]
Carbon Disulfide	Acetone	328.7	3.50	3.64	4.0%	3.70	5.7%	[17]
Carbon Disulfide	Acetonitrile	293.2	12.40	10.26	-17.3%	12.97	4.6%	[10]
Carbon Disulfide	Acetophenone	293.2	2.05	2.02	-1.5%	2.13	3.9%	[10]
Carbon Disulfide	Aniline	293.2	3.53	3.73	5.7%	M.P.	N.A.	[10]
Carbon Disulfide	Anisole	293.2	1.62	1.58	-2.5%	1.52	-6.2%	[10]
Carbon Disulfide	Benzene	293.2	1.49	1.37	-8.1%	1.56	4.7%	[58]
Carbon Disulfide	Benzene	293.2	1.48	1.37	-7.4%	1.56	5.4%	[10]
Carbon Disulfide	Benzonitrile	293.2	2.33	2.59	11.2%	M.G.	N.A.	[10]
Carbon Disulfide	Carbon Tetrachloride	293.2	1.21	1.19	-1.7%	1.24	2.5%	[10]
Carbon Disulfide	Cyclohexanone	293.2	1.87	1.85	-1.1%	1.66	-11.2%	[10]
Carbon Disulfide	Ethyl Acetate	293.2	2.66	2.41	-9.4%	2.59	-2.6%	[10]
Carbon Disulfide	Methyl Ethyl Ketone	293.2	3.04	2.56	-15.8%	2.99	-1.6%	[10]
Carbon Disulfide	N,N-Dimethylformamide	293.2	4.36	3.76	-13.8%	M.P.	N.A.	[10]
Carbon Disulfide	N-Heptane	293.2	1.30	1.29	-0.8%	1.41	8.5%	[10]
Carbon Disulfide	Nitrobenzene	293.2	2.63	2.48	-5.7%	M.P.	N.A.	[10]
Carbon Disulfide	Nitroethane	293.2	5.03	5.00	-0.6%	7.31	45.3%	[10]
Carbon Disulfide	Nitromethane	293.2	15.10	13.16	-12.8%	37.02	145.2%	[10]
Carbon Disulfide	N-Octane	293.2	1.26	1.17	-7.1%	1.27	0.8%	[10]
Carbon Disulfide	Phenol	323.2	3.20	3.12	-2.5%	M.P.	N.A.	[10]
Carbon Disulfide	Propionitrile	293.2	5.51	4.60	-16.5%	4.81	-12.7%	[10]
Carbon Disulfide	P-Xylene	293.2	1.07	1.20	12.1%	1.10	2.8%	[10]
Carbon Disulfide	Toluene	293.2	1.27	1.22	-3.9%	1.27	0.0%	[10]
Carbon Disulfide	Tributyl Phosphate	298.2	1.01	0.81	-19.8%	M.G.	N.A.	[20]
Carbon Disulfide	Tributyl Phosphate	318.2	0.90	0.79	-12.2%	M.G.	N.A.	[20]
Carbon Disulfide	Tributyl Phosphate	333.2	0.84	0.77	-8.3%	M.G.	N.A.	[20]
Carbon Tetrachloride	1,1,1-Trichloroethane	328.2	1.08	1.06	-1.9%	1.06	-1.9%	[1]
Carbon Tetrachloride	1,2-Dichloroethane	293.2	1.98	1.77	-10.6%	1.51	-23.7%	[10]
Carbon Tetrachloride	1,2-Dichloroethane	306.9	1.86	1.70	-8.6%	1.45	-22.0%	[12]
Carbon Tetrachloride	1,2-Dichloroethane	313.2	1.82	1.67	-8.3%	1.42	-22.0%	408
Carbon Tetrachloride	1,2-Dichloroethane	318.4	1.76	1.64	-6.8%	1.40	-20.5%	[12]
Carbon Tetrachloride	1,2-Dichloroethane	328.2	1.79	1.60	-10.6%	1.37	-23.5%	[1]
Carbon Tetrachloride	1,2-Dichloroethane	337.2	1.65	1.57	-4.8%	1.34	-18.8%	[12]
Carbon Tetrachloride	1,2-Dichloroethane	355.0	1.55	1.52	-1.9%	1.29	-16.8%	[12]
Carbon Tetrachloride	1,4-Dioxane	298.2	1.28	1.31	2.0%	1.13	-12.0%	32
Carbon Tetrachloride	1,4-Dioxane	303.2	1.28	1.30	1.9%	1.14	-10.6%	32
Carbon Tetrachloride	1,4-Dioxane	308.2	1.33	1.30	-2.2%	1.15	-13.4%	32
Carbon Tetrachloride	1,4-Dioxane	313.2	1.38	1.30	-6.0%	1.15	-16.8%	32
Carbon Tetrachloride	1,4-Dioxane	313.2	1.16	1.30	12.1%	1.15	-0.9%	[15]
Carbon Tetrachloride	1,4-Dioxane	337.7	1.19	1.28	7.6%	1.18	-0.8%	[15]
Carbon Tetrachloride	1-Butanol	293.2	2.67	2.85	6.7%	2.83	6.0%	[10]
Carbon Tetrachloride	1-Butanol	359.6	2.58	2.46	-4.7%	2.77	7.4%	[17]
Carbon Tetrachloride	1-Hexanol	293.2	2.01	2.27	12.9%	2.10	4.5%	[28]
Carbon Tetrachloride	1-Hexanol	313.2	1.98	2.19	10.6%	2.06	4.0%	[28]

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Carbon Tetrachloride	1-Hexanol	333.2	1.94	2.10	8.2%	2.04	5.2%	[28]
Carbon Tetrachloride	1-Octanol	293.2	1.74	1.61	-7.5%	1.71	-1.7%	[10]
Carbon Tetrachloride	1-Octanol	298.2	1.83	1.60	-12.6%	1.70	-7.1%	[2]
Carbon Tetrachloride	1-Octanol	298.2	1.67	1.60	-4.2%	1.70	1.8%	[3]
Carbon Tetrachloride	1-Octanol	298.2	1.83	1.60	-12.6%	1.70	-7.1%	[4]
Carbon Tetrachloride	1-Octanol	303.2	1.71	1.58	-7.6%	1.69	-1.2%	[2]
Carbon Tetrachloride	1-Octanol	313.2	1.69	1.55	-8.3%	1.67	-1.2%	[2]
Carbon Tetrachloride	1-Phenyl-1-Butanone	298.1	1.33	1.19	-10.5%	1.30	-2.3%	[34]
Carbon Tetrachloride	1-Propanol	332.9	3.20	3.43	7.2%	3.58	11.9%	[17]
Carbon Tetrachloride	1-Propanol	343.1	3.14	3.32	5.7%	3.57	13.7%	[17]
Carbon Tetrachloride	1-Propanol	352.4	3.10	3.23	4.2%	3.56	14.8%	[17]
Carbon Tetrachloride	1-Propanol	362.4	3.10	3.12	0.6%	3.53	13.9%	[17]
Carbon Tetrachloride	1-Propanol	369.9	3.02	3.05	1.0%	3.49	15.6%	[17]
Carbon Tetrachloride	2-Nitropropane	293.2	2.40	2.77	15.4%	2.15	-10.4%	[10]
Carbon Tetrachloride	Acetone	300.9	2.09	2.34	12.0%	2.07	-1.0%	[17]
Carbon Tetrachloride	Acetone	304.0	2.16	2.32	7.4%	2.07	-4.2%	[12]
Carbon Tetrachloride	Acetone	306.9	2.07	2.30	11.1%	2.07	0.0%	[17]
Carbon Tetrachloride	Acetone	310.9	2.13	2.27	6.6%	2.06	-3.3%	[12]
Carbon Tetrachloride	Acetone	313.9	2.07	2.25	8.7%	2.06	-0.5%	[17]
Carbon Tetrachloride	Acetone	319.5	2.07	2.22	7.2%	2.06	-0.5%	[17]
Carbon Tetrachloride	Acetone	324.4	2.03	2.19	7.9%	2.05	1.0%	[17]
Carbon Tetrachloride	Acetone	326.0	2.15	2.18	1.4%	2.05	-4.7%	[12]
Carbon Tetrachloride	Acetone	327.6	2.13	2.17	1.9%	2.05	-3.8%	[12]
Carbon Tetrachloride	Acetone	328.4	2.04	2.16	5.9%	2.04	0.0%	[17]
Carbon Tetrachloride	Acetone	329.4	2.15	2.16	0.5%	2.04	-5.1%	[11]
Carbon Tetrachloride	Acetone	329.4	2.10	2.16	2.9%	2.04	-2.9%	[11]
Carbon Tetrachloride	Acetonitrile	293.2	6.67	8.30	24.4%	5.70	-14.5%	[10]
Carbon Tetrachloride	Acetonitrile	352.6	4.90	4.60	-6.1%	4.58	-6.5%	[12]
Carbon Tetrachloride	Acetophenone	293.2	1.70	1.80	5.9%	2.07	21.8%	[10]
Carbon Tetrachloride	Aniline	293.2	4.80	4.61	-4.0%	4.08	-15.0%	[10]
Carbon Tetrachloride	Anisole	293.2	1.54	1.37	-11.0%	0.79	-48.7%	[5]
Carbon Tetrachloride	Anisole	293.2	1.30	1.37	5.4%	0.79	-39.2%	[10]
Carbon Tetrachloride	Benzene	293.2	1.13	1.10	-2.7%	1.15	1.8%	[58]
Carbon Tetrachloride	Benzene	293.2	1.13	1.10	-2.7%	1.15	1.8%	[10]
Carbon Tetrachloride	Benzene	313.2	1.13	1.09	-3.8%	1.13	-0.3%	91
Carbon Tetrachloride	Benzene	353.3	1.15	1.08	-6.1%	1.10	-4.3%	[11]
Carbon Tetrachloride	Benzyl Acetate	298.2	1.41	1.52	7.8%	1.13	-19.9%	[10]
Carbon Tetrachloride	Butyl Ether	293.2	0.77	0.76	-1.3%	0.84	9.1%	[5]
Carbon Tetrachloride	Butyl Ether	308.2	0.83	0.78	-6.2%	0.85	2.2%	134
Carbon Tetrachloride	Chloroform	293.2	1.21	1.17	-3.6%	1.19	-2.0%	252
Carbon Tetrachloride	Chloroform	303.2	1.20	1.17	-2.6%	1.18	-1.8%	252
Carbon Tetrachloride	Chloroform	328.2	1.16	1.15	-0.9%	1.14	-1.7%	[1]
Carbon Tetrachloride	Cyclohexane	343.2	1.08	1.13	4.7%	1.04	-3.7%	315
Carbon Tetrachloride	Cyclohexanone	293.2	1.10	1.23	11.8%	1.27	15.5%	[10]
Carbon Tetrachloride	Dichloromethane	308.2	1.66	1.52	-8.4%	1.64	-1.2%	[1]
Carbon Tetrachloride	Di-N-Propyl Ether	298.2	0.91	1.00	10.4%	0.88	-2.9%	139
Carbon Tetrachloride	Ethanol	298.2	5.14	5.63	9.5%	4.98	-3.1%	[30]
Carbon Tetrachloride	Ethanol	313.2	4.43	5.41	22.1%	5.02	13.3%	[28]
Carbon Tetrachloride	Ethanol	333.2	4.05	5.04	24.4%	5.07	25.2%	[28]
Carbon Tetrachloride	Ethyl Acetate	293.2	1.31	1.42	8.4%	1.25	-4.6%	[10]
Carbon Tetrachloride	Ethyl Acetate	329.2	1.28	1.38	7.8%	1.27	-0.8%	[12]
Carbon Tetrachloride	Isopropanol	354.8	3.41	3.17	-7.0%	3.24	-5.0%	[17]

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Carbon Tetrachloride	Methanol	293.2	7.48	10.67	42.6%	7.75	3.6%	[28]
Carbon Tetrachloride	Methanol	298.2	7.58	10.51	38.7%	7.77	2.5%	[30]
Carbon Tetrachloride	Methanol	313.2	7.22	9.89	37.0%	7.80	8.0%	[28]
Carbon Tetrachloride	Methanol	333.2	6.52	8.87	36.0%	7.77	19.2%	[28]
Carbon Tetrachloride	Methyl Ethyl Ketone	293.2	1.65	1.50	-9.1%	1.70	3.0%	[10]
Carbon Tetrachloride	Methyl Isobutyl Ketone	293.2	1.05	1.07	1.9%	1.33	26.7%	[5]
Carbon Tetrachloride	N,N-Dibutylformamide	302.8	0.89	0.79	-11.2%	1.03	15.7%	[13]
Carbon Tetrachloride	N,N-Dibutylformamide	318.3	0.90	0.81	-10.2%	1.05	16.4%	[13]
Carbon Tetrachloride	N,N-Dibutylformamide	332.4	0.92	0.82	-10.8%	1.06	15.3%	[13]
Carbon Tetrachloride	N,N-Dimethylacetamide	303.2	0.95	1.80	89.7%	M.P.	N.A.	[13]
Carbon Tetrachloride	N,N-Dimethylacetamide	317.6	1.23	1.76	43.0%	M.P.	N.A.	[13]
Carbon Tetrachloride	N,N-Dimethylacetamide	333.6	1.62	1.72	6.4%	M.P.	N.A.	[13]
Carbon Tetrachloride	N-Decane	313.2	0.99	0.99	-0.1%	1.01	1.9%	92
Carbon Tetrachloride	N-Heptane	293.2	1.20	1.19	-0.8%	1.18	-1.7%	[10]
Carbon Tetrachloride	N-Heptane	313.2	1.15	1.16	0.9%	1.15	0.1%	94
Carbon Tetrachloride	N-Hexadecane	298.2	0.83	0.79	-4.9%	0.85	2.3%	[6]
Carbon Tetrachloride	N-Hexane	301.0	1.20	1.25	4.2%	1.23	2.5%	[12]
Carbon Tetrachloride	N-Hexane	313.2	1.20	1.23	2.2%	1.21	0.6%	95
Carbon Tetrachloride	N-Hexane	315.0	1.20	1.23	2.5%	1.21	0.8%	[12]
Carbon Tetrachloride	N-Hexane	332.0	1.19	1.21	1.7%	1.19	0.0%	[12]
Carbon Tetrachloride	N-Hexane	340.3	1.16	1.20	3.4%	1.18	1.7%	[12]
Carbon Tetrachloride	Nitrobenzene	293.2	2.26	2.35	4.0%	2.27	0.4%	[10]
Carbon Tetrachloride	Nitroethane	293.2	3.93	4.06	3.3%	2.91	-26.0%	[10]
Carbon Tetrachloride	Nitromethane	293.2	8.81	11.77	33.6%	7.66	-13.1%	[10]
Carbon Tetrachloride	N-Methylacetamide	304.2	2.99	3.82	27.8%	M.P.	N.A.	[13]
Carbon Tetrachloride	N-Methylacetamide	318.4	3.15	3.65	16.0%	M.P.	N.A.	[13]
Carbon Tetrachloride	N-Methylacetamide	331.9	3.29	3.48	5.7%	M.P.	N.A.	[13]
Carbon Tetrachloride	N-Octane	293.2	1.17	1.12	-4.3%	1.13	-3.4%	[74]
Carbon Tetrachloride	N-Octane	313.2	1.08	1.10	1.6%	1.09	0.7%	93
Carbon Tetrachloride	Phenol	323.2	3.40	3.97	16.8%	4.08	20.0%	[10]
Carbon Tetrachloride	Phenol	328.2	4.56	3.91	-14.3%	4.07	-10.7%	[14]
Carbon Tetrachloride	Phenol	343.2	4.19	3.72	-11.2%	4.04	-3.6%	[14]
Carbon Tetrachloride	Phenol	358.2	4.08	3.52	-13.7%	4.02	-1.5%	[14]
Carbon Tetrachloride	Phenol	373.2	3.89	3.33	-14.4%	4.02	3.3%	[14]
Carbon Tetrachloride	Propionitrile	293.2	3.14	3.68	17.2%	3.08	-1.9%	[10]
Carbon Tetrachloride	P-Xylene	293.2	0.93	0.96	3.2%	0.90	-3.2%	[10]
Carbon Tetrachloride	Quinoline	298.2	1.44	1.83	27.1%	M.G.	N.A.	[10]
Carbon Tetrachloride	Sulfolane	303.3	4.60	6.70	45.6%	M.G.	N.A.	[13]
Carbon Tetrachloride	Sulfolane	317.9	4.58	5.78	26.1%	M.G.	N.A.	[13]
Carbon Tetrachloride	Sulfolane	333.7	4.56	5.02	10.0%	M.G.	N.A.	[13]
Carbon Tetrachloride	Tetrahydrofuran	303.2	0.77	0.84	9.1%	0.90	16.9%	300
Carbon Tetrachloride	Toluene	293.2	1.02	1.02	0.0%	1.00	-2.0%	[10]
Carbon Tetrachloride	Toluene	313.2	1.07	1.02	-5.1%	1.00	-7.0%	90
Carbon Tetrachloride	Tributyl Phosphate	298.2	0.63	0.52	-17.5%	M.G.	N.A.	[20]
Carbon Tetrachloride	Tributyl Phosphate	298.2	0.51	0.52	2.0%	M.G.	N.A.	[8]
Carbon Tetrachloride	Tributyl Phosphate	298.6	0.59	0.52	-11.9%	M.G.	N.A.	[27]
Carbon Tetrachloride	Tributyl Phosphate	302.9	0.62	0.52	-16.1%	M.G.	N.A.	[27]
Carbon Tetrachloride	Tributyl Phosphate	303.2	0.53	0.52	-1.9%	M.G.	N.A.	[8]
Carbon Tetrachloride	Tributyl Phosphate	308.2	0.53	0.53	0.0%	M.G.	N.A.	[8]
Carbon Tetrachloride	Tributyl Phosphate	308.6	0.64	0.53	-17.2%	M.G.	N.A.	[27]
Carbon Tetrachloride	Tributyl Phosphate	313.1	0.65	0.53	-18.5%	M.G.	N.A.	[27]
Carbon Tetrachloride	Tributyl Phosphate	313.2	0.54	0.53	-1.9%	M.G.	N.A.	[8]

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Carbon Tetrachloride	Tributyl Phosphate	318.2	0.63	0.54	-14.3%	M.G.	N.A.	[20]
Carbon Tetrachloride	Tributyl Phosphate	318.2	0.54	0.54	0.0%	M.G.	N.A.	[8]
Carbon Tetrachloride	Tributyl Phosphate	323.2	0.56	0.54	-3.6%	M.G.	N.A.	[8]
Carbon Tetrachloride	Tributyl Phosphate	323.7	0.64	0.54	-15.6%	M.G.	N.A.	[27]
Carbon Tetrachloride	Tributyl Phosphate	333.2	0.64	0.55	-14.1%	M.G.	N.A.	[20]
Carbon Tetrachloride	Tributyl Phosphate	363.2	0.67	0.58	-13.4%	M.G.	N.A.	[20]
Carbon Tetrachloride	Tributyl Phosphate	373.2	0.68	0.58	-14.7%	M.G.	N.A.	[20]
Carbon Tetrachloride	Trichloroethylene	328.2	0.99	1.04	5.1%	0.93	-6.1%	[9]
Chlorobenzene	1-Nitropropane	353.5	1.35	1.42	5.2%	1.53	13.3%	[12]
Chlorobenzene	Acetone	313.2	1.58	1.79	13.4%	1.44	-8.8%	39
Chlorobenzene	Acetone	353.2	1.56	1.64	5.3%	1.38	-11.4%	39
Chlorobenzene	Acetone	386.7	1.55	1.55	-0.3%	1.29	-17.0%	39
Chlorobenzene	Acetonitrile	293.2	4.32	3.70	-14.4%	4.74	9.6%	131
Chlorobenzene	Acetonitrile	328.2	4.15	2.90	-30.1%	3.97	-4.3%	131
Chlorobenzene	Acetonitrile	343.2	3.66	2.66	-27.4%	3.69	0.7%	131
Chlorobenzene	Acetonitrile	393.2	3.16	2.11	-33.3%	2.91	-7.9%	131
Chlorobenzene	Aniline	293.2	2.59	2.25	-13.1%	1.70	-34.4%	370
Chlorobenzene	Aniline	343.2	2.08	1.90	-8.5%	1.54	-25.8%	370
Chlorobenzene	Aniline	393.2	1.79	1.67	-6.7%	1.43	-20.1%	370
Chlorobenzene	Cyclohexane	348.2	1.58	1.53	-3.2%	1.45	-8.3%	56
Chlorobenzene	Dichloromethane	298.0	1.11	0.84	-24.6%	1.16	4.1%	147
Chlorobenzene	Dichloromethane	348.0	1.11	0.86	-22.2%	1.10	-0.5%	147
Chlorobenzene	Dichloromethane	398.1	1.07	0.88	-18.0%	1.11	3.5%	147
Chlorobenzene	Ethanol	323.2	5.20	5.54	6.5%	4.36	-16.2%	[12]
Chlorobenzene	Ethanol	335.8	5.10	5.26	3.1%	4.24	-16.9%	[12]
Chlorobenzene	Ethanol	348.0	4.90	4.98	1.6%	4.11	-16.1%	[12]
Chlorobenzene	Ethyl Acetate	313.2	1.08	1.28	18.6%	0.94	-12.9%	39
Chlorobenzene	Ethyl Acetate	353.2	1.12	1.24	10.8%	1.07	-4.4%	39
Chlorobenzene	Ethyl Acetate	393.2	1.14	1.21	6.6%	1.09	-4.0%	39
Chlorobenzene	Ethylbenzene	293.2	0.99	1.02	2.7%	1.05	5.7%	39
Chlorobenzene	Methanol	328.2	8.75	8.20	-6.3%	9.59	9.6%	132
Chlorobenzene	N,N-Dimethylacetamide	317.6	3.31	1.55	-53.1%	M.P.	N.A.	[13]
Chlorobenzene	N-Methylacetamide	332.8	3.06	3.36	9.7%	M.P.	N.A.	[13]
Chlorobenzene	Sulfolane	303.8	2.69	3.24	20.4%	M.G.	N.A.	[13]
Chlorobenzene	Sulfolane	317.9	2.60	2.96	14.1%	M.G.	N.A.	[13]
Chlorobenzene	Sulfolane	332.8	2.47	2.71	9.9%	M.G.	N.A.	[13]
Chlorobenzene	Tetraethylene Glycol DME	313.2	0.59	0.94	58.2%	0.61	2.7%	[7]
Chlorobenzene	Tetraethylene Glycol DME	327.6	0.62	0.93	49.0%	0.64	2.6%	[7]
Chlorobenzene	Tetraethylene Glycol DME	343.2	0.66	0.93	40.7%	0.67	1.4%	[7]
Chloroform	1,1,1-Trichloroethane	328.2	0.97	0.97	0.0%	M.P.	N.A.	[1]
Chloroform	1,2-Dichloroethane	293.2	1.06	1.01	-4.7%	0.86	-18.9%	[10]
Chloroform	1,2-Dichloroethane	328.2	1.03	1.02	-1.0%	0.86	-16.5%	[1]
Chloroform	1,4-Dioxane	303.2	0.37	0.32	-13.3%	0.32	-13.3%	210
Chloroform	1,4-Dioxane	323.2	0.41	0.37	-10.5%	0.36	-12.9%	210
Chloroform	1-Butanol	293.2	1.20	1.61	34.2%	1.51	25.8%	[10]
Chloroform	1-Butanol	308.2	1.32	1.58	19.7%	1.53	15.9%	[30]
Chloroform	1-Butanol	318.2	1.40	1.56	11.4%	1.54	10.0%	[30]
Chloroform	1-Butanol	328.2	1.38	1.54	11.6%	1.54	11.6%	[30]
Chloroform	1-Chlorobutane	293.2	0.93	0.84	-9.7%	0.89	-4.3%	[10]
Chloroform	1-Octanol	293.2	0.95	0.92	-3.2%	1.26	32.6%	[10]
Chloroform	1-Octanol	298.2	1.02	0.91	-10.8%	1.25	22.5%	[2]
Chloroform	1-Octanol	298.2	0.97	0.91	-6.2%	1.25	28.9%	[3]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Chloroform	1-Octanol	298.2	1.02	0.91	-10.8%	1.25	22.5%	[4]
Chloroform	1-Octanol	308.2	1.03	0.91	-11.7%	1.23	19.4%	[2]
Chloroform	1-Octanol	323.2	1.07	0.90	-15.9%	1.19	11.2%	[2]
Chloroform	1-Pentanol	308.2	1.46	1.52	4.1%	1.44	-1.4%	[30]
Chloroform	1-Pentanol	318.2	1.29	1.49	15.5%	1.43	10.9%	[30]
Chloroform	1-Pentanol	328.2	1.32	1.47	11.4%	1.42	7.6%	[30]
Chloroform	1-Phenyl-1-Butanone	298.1	0.50	0.42	-16.0%	0.23	-54.0%	[34]
Chloroform	2,2,4-Trimethylpentane	293.2	1.51	1.72	13.9%	1.45	-4.0%	[10]
Chloroform	2-Nitropropane	293.2	0.88	0.91	3.4%	M.P.	N.A.	[10]
Chloroform	2-Pyrrolidone	303.2	0.53	0.82	53.6%	M.G.	N.A.	[35]
Chloroform	2-Pyrrolidone	313.2	0.59	0.82	38.7%	M.G.	N.A.	[35]
Chloroform	2-Pyrrolidone	323.2	0.65	0.82	25.6%	M.G.	N.A.	[35]
Chloroform	2-Pyrrolidone	333.2	0.71	0.82	15.0%	M.G.	N.A.	[35]
Chloroform	Acetone	307.2	0.50	0.42	-16.0%	0.44	-12.0%	[17]
Chloroform	Acetone	313.9	0.51	0.44	-13.7%	0.46	-9.8%	[17]
Chloroform	Acetone	319.5	0.51	0.46	-9.8%	0.48	-5.9%	[17]
Chloroform	Acetone	323.2	0.55	0.47	-14.3%	0.49	-10.7%	213
Chloroform	Acetone	324.4	0.52	0.48	-7.7%	0.49	-5.8%	[17]
Chloroform	Acetone	328.5	0.53	0.49	-7.5%	0.51	-3.8%	[17]
Chloroform	Acetone	329.4	0.63	0.49	-22.2%	0.51	-19.0%	[11]
Chloroform	Acetonitrile	293.2	1.49	1.57	5.4%	1.21	-18.8%	[10]
Chloroform	Acetonitrile	298.2	1.29	1.55	20.2%	1.23	-4.7%	[36]
Chloroform	Acetonitrile	318.1	1.32	1.48	12.1%	1.27	-3.8%	[60]
Chloroform	Acetonitrile	328.3	1.31	1.45	10.7%	1.29	-1.5%	[60]
Chloroform	Acetophenone	293.2	0.58	0.55	-5.2%	0.20	-65.5%	[10]
Chloroform	Aniline	293.2	1.50	1.51	0.7%	M.P.	N.A.	[10]
Chloroform	Anisole	293.2	0.88	0.60	-31.8%	0.03	-96.6%	[5]
Chloroform	Anisole	293.2	0.68	0.60	-11.8%	0.03	-95.6%	[10]
Chloroform	Benzene	293.2	0.81	0.75	-7.4%	0.83	2.5%	[10]
Chloroform	Benzene	353.3	0.87	0.84	-3.4%	0.86	-1.1%	[11]
Chloroform	Benzene	353.3	0.88	0.84	-4.5%	0.86	-2.3%	[11]
Chloroform	Benzyl Acetate	298.2	0.51	0.50	-2.0%	0.11	-78.4%	[10]
Chloroform	Butyl Ether	293.2	0.47	0.40	-14.9%	0.45	-4.3%	[5]
Chloroform	Carbon Tetrachloride	293.2	1.19	1.17	-1.7%	1.19	0.0%	252
Chloroform	Carbon Tetrachloride	293.2	1.16	1.17	0.9%	1.19	2.6%	[10]
Chloroform	Carbon Tetrachloride	303.2	1.17	1.16	-0.6%	1.17	0.3%	252
Chloroform	Carbon Tetrachloride	328.2	1.13	1.14	0.9%	1.14	0.9%	[1]
Chloroform	Cyclohexanone	293.2	0.31	0.24	-22.6%	0.40	29.0%	[10]
Chloroform	Dichloromethane	308.2	1.05	1.00	-4.8%	1.06	1.0%	[1]
Chloroform	Diethyl Phthalate	303.2	0.42	0.39	-8.0%	M.G.	N.A.	[39]
Chloroform	Diethyl Phthalate	313.2	0.45	0.41	-7.9%	M.G.	N.A.	[39]
Chloroform	Diethyl Phthalate	323.2	0.47	0.42	-10.3%	M.G.	N.A.	[39]
Chloroform	Diethyl Phthalate	333.2	0.49	0.44	-10.2%	M.G.	N.A.	[39]
Chloroform	Dimethyl Sulfoxide	293.2	0.24	0.18	-24.3%	0.41	72.5%	302
Chloroform	Dimethyl Sulfoxide	298.2	0.26	0.19	-26.6%	0.43	66.2%	302
Chloroform	Dimethyl Sulfoxide	308.2	0.30	0.23	-23.6%	0.47	56.1%	302
Chloroform	Dimethyl Sulfoxide	318.2	0.35	0.26	-25.1%	0.51	46.9%	302
Chloroform	Dimethyl Sulfoxide	328.2	0.40	0.30	-24.4%	0.55	38.6%	302
Chloroform	Di-N-Propyl Ether	298.2	0.42	0.39	-7.8%	0.43	1.7%	140
Chloroform	Epsilon-Caprolactone	303.2	0.40	0.44	8.9%	M.G.	N.A.	[41]
Chloroform	Epsilon-Caprolactone	318.2	0.45	0.48	7.1%	M.G.	N.A.	[41]
Chloroform	Epsilon-Caprolactone	333.2	0.50	0.53	6.9%	M.G.	N.A.	[41]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Chloroform	Ethanol	298.2	1.71	2.56	49.7%	1.75	2.3%	[30]
Chloroform	Ethanol	323.2	2.15	2.46	14.3%	1.93	-10.3%	201
Chloroform	Ethanol	323.2	2.14	2.46	15.1%	1.93	-9.7%	201
Chloroform	Ethyl Acetate	310.5	0.42	0.42	0.0%	0.45	7.1%	[17]
Chloroform	Ethyl Acetate	313.2	0.42	0.42	0.0%	0.45	7.1%	231
Chloroform	Ethyl Acetate	323.2	0.44	0.45	2.1%	0.48	8.9%	231
Chloroform	Ethyl Acetate	327.2	0.47	0.46	-2.1%	0.49	4.3%	[17]
Chloroform	Ethyl Acetate	329.2	0.52	0.47	-9.6%	0.49	-5.8%	[12]
Chloroform	Ethyl Acetate	340.0	0.50	0.50	0.0%	0.51	2.0%	[17]
Chloroform	Ethyl Acetate	349.2	0.49	0.52	6.1%	0.52	6.1%	[12]
Chloroform	Ethyl Acetate	349.5	0.51	0.52	2.0%	0.52	2.0%	[17]
Chloroform	Glutaronitrile	303.2	1.59	1.88	18.2%	M.G.	N.A.	[39]
Chloroform	Glutaronitrile	313.2	1.63	1.82	11.7%	M.G.	N.A.	[39]
Chloroform	Glutaronitrile	323.2	1.69	1.76	4.1%	M.G.	N.A.	[39]
Chloroform	Glutaronitrile	333.2	1.73	1.71	-1.2%	M.G.	N.A.	[39]
Chloroform	Isopropanol	323.2	1.95	1.82	-6.5%	1.62	-16.7%	234
Chloroform	Methanol	293.2	2.21	4.05	83.3%	2.20	-0.5%	261
Chloroform	Methanol	298.2	2.34	4.02	71.8%	2.26	-3.4%	[30]
Chloroform	Methanol	303.2	2.28	3.98	74.6%	2.32	1.8%	261
Chloroform	Methanol	317.7	2.43	3.84	58.0%	2.48	2.1%	[60]
Chloroform	Methanol	323.2	2.85	3.78	32.8%	2.53	-11.1%	261
Chloroform	Methanol	328.2	2.39	3.71	55.2%	2.58	7.9%	[60]
Chloroform	Methyl Acetate	312.9	0.52	0.53	1.9%	0.48	-7.7%	[60]
Chloroform	Methyl Acetate	322.7	0.56	0.56	0.0%	0.51	-8.9%	[60]
Chloroform	Methyl Ethyl Ketone	318.2	0.37	0.37	-0.3%	0.48	29.4%	232
Chloroform	Methyl Ethyl Ketone	328.2	0.39	0.40	2.9%	0.51	31.2%	232
Chloroform	Methyl Isobutyl Ketone	293.2	0.37	0.34	-8.1%	0.42	13.5%	[5]
Chloroform	N,N-Dibutylformamide	302.8	0.16	0.12	-24.5%	M.P.	N.A.	[13]
Chloroform	N,N-Dibutylformamide	318.3	0.19	0.15	-21.5%	M.P.	N.A.	[13]
Chloroform	N,N-Dibutylformamide	332.4	0.22	0.18	-19.3%	M.P.	N.A.	[13]
Chloroform	N,N-Diethylacetamide	303.2	0.13	0.12	-7.0%	M.P.	N.A.	[39]
Chloroform	N,N-Diethylacetamide	313.2	0.15	0.14	-5.4%	M.P.	N.A.	[39]
Chloroform	N,N-Diethylacetamide	323.2	0.17	0.16	-7.0%	M.P.	N.A.	[39]
Chloroform	N,N-Diethylacetamide	333.2	0.19	0.18	-4.3%	M.P.	N.A.	[39]
Chloroform	N,N-Dimethylacetamide	303.2	0.18	0.16	-10.1%	M.P.	N.A.	[13]
Chloroform	N,N-Dimethylacetamide	317.6	0.22	0.19	-12.4%	M.P.	N.A.	[13]
Chloroform	N,N-Dimethylacetamide	333.2	0.27	0.23	-16.1%	M.P.	N.A.	[13]
Chloroform	N-Ethylacetamide	303.2	0.48	0.70	46.4%	M.G.	N.A.	[39]
Chloroform	N-Ethylacetamide	313.2	0.53	0.70	32.8%	M.G.	N.A.	[39]
Chloroform	N-Ethylacetamide	323.2	0.59	0.71	20.7%	M.G.	N.A.	[39]
Chloroform	N-Ethylacetamide	333.2	0.65	0.71	10.1%	M.G.	N.A.	[39]
Chloroform	N-Heptane	293.2	1.47	1.68	14.3%	1.54	4.8%	[10]
Chloroform	N-Heptane	293.2	1.47	1.68	14.3%	1.54	4.8%	[10]
Chloroform	N-Heptane	323.2	1.38	1.51	9.1%	1.38	-0.3%	321
Chloroform	N-Hexadecane	298.2	1.06	1.16	10.0%	1.04	-1.4%	[6]
Chloroform	N-Hexane	301.0	1.58	1.72	8.9%	1.59	0.6%	[12]
Chloroform	N-Hexane	301.9	1.56	1.71	9.6%	1.59	1.9%	[17]
Chloroform	N-Hexane	308.2	1.51	1.67	10.5%	1.55	2.5%	265
Chloroform	N-Hexane	315.3	1.53	1.63	6.5%	1.52	-0.7%	[12]
Chloroform	N-Hexane	317.7	1.54	1.62	5.2%	1.50	-2.6%	[17]
Chloroform	N-Hexane	318.2	1.47	1.62	10.3%	1.50	2.1%	265
Chloroform	N-Hexane	328.2	1.41	1.57	11.0%	1.45	2.5%	265

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Chloroform	N-Hexane	331.8	1.48	1.55	4.7%	1.44	-2.7%	[12]
Chloroform	N-Hexane	334.7	1.46	1.54	5.5%	1.43	-2.1%	[17]
Chloroform	N-Hexane	340.1	1.39	1.52	9.4%	1.40	0.7%	[12]
Chloroform	N-Hexane	340.6	1.42	1.51	6.3%	1.40	-1.4%	[17]
Chloroform	N-Hexane	342.0	1.41	1.51	7.1%	1.40	-0.7%	[11]
Chloroform	N-Hexane	342.0	1.44	1.51	4.9%	1.40	-2.8%	[11]
Chloroform	Nitrobenzene	293.2	1.02	0.86	-15.7%	M.P.	N.A.	[10]
Chloroform	Nitroethane	293.2	1.00	1.08	8.0%	M.P.	N.A.	[10]
Chloroform	Nitromethane	293.2	2.20	2.35	6.8%	M.P.	N.A.	[10]
Chloroform	N-Methyl-2-Pyrrolidone	323.2	0.04	0.17	286.5%	M.P.	N.A.	323
Chloroform	N-Methyl-2-Pyrrolidone	373.2	0.09	0.30	222.9%	M.P.	N.A.	323
Chloroform	N-Methylacetamide	303.1	0.56	0.94	67.0%	M.P.	N.A.	[13]
Chloroform	N-Methylacetamide	318.4	0.73	0.94	28.1%	M.P.	N.A.	[13]
Chloroform	N-Methylacetamide	333.1	0.75	0.94	25.0%	M.P.	N.A.	[13]
Chloroform	N-Methylformamide	303.2	1.16	1.81	56.7%	M.P.	N.A.	[35]
Chloroform	N-Methylformamide	313.2	1.24	1.78	43.4%	M.P.	N.A.	[35]
Chloroform	N-Methylformamide	323.2	1.32	1.74	31.4%	M.P.	N.A.	[35]
Chloroform	N-Methylformamide	333.2	1.41	1.71	21.1%	M.P.	N.A.	[35]
Chloroform	N-Octane	293.2	1.43	1.61	12.6%	1.45	1.4%	[10]
Chloroform	N-Octane	313.2	1.55	1.49	-3.9%	1.35	-12.9%	[36]
Chloroform	N-Octane	333.2	1.43	1.40	-2.1%	1.27	-11.2%	[36]
Chloroform	Phenol	323.2	1.75	2.60	48.6%	M.P.	N.A.	[10]
Chloroform	Propionitrile	293.2	0.89	0.87	-2.2%	0.87	-2.2%	[10]
Chloroform	Pyridine	303.2	0.40	0.38	-4.4%	0.12	-69.8%	293
Chloroform	Quinoline	298.2	0.47	0.50	6.4%	M.G.	N.A.	[10]
Chloroform	Sulfolane	303.1	0.93	0.97	3.9%	M.G.	N.A.	[13]
Chloroform	Sulfolane	317.9	0.97	0.98	0.6%	M.G.	N.A.	[13]
Chloroform	Sulfolane	332.6	1.01	1.00	-0.6%	M.G.	N.A.	[13]
Chloroform	Tetraethylene Glycol DME	303.2	0.16	0.15	-4.5%	0.18	14.6%	[7]
Chloroform	Tetraethylene Glycol DME	323.2	0.20	0.19	-5.0%	0.21	5.0%	[7]
Chloroform	Tetraethylene Glycol DME	343.2	0.26	0.22	-16.0%	0.23	-12.2%	[7]
Chloroform	Tetrahydrofuran	303.2	0.19	0.20	3.7%	0.32	65.9%	298
Chloroform	Tetrahydrofuran	313.2	0.23	0.23	0.0%	0.35	52.2%	[15]
Chloroform	Tetrahydrofuran	313.6	0.35	0.23	-34.3%	0.35	0.0%	[60]
Chloroform	Tetrahydrofuran	323.2	0.26	0.26	0.0%	0.38	46.2%	[15]
Chloroform	Tetrahydrofuran	323.3	0.37	0.26	-29.7%	0.38	2.7%	[60]
Chloroform	Tetrahydrofuran	327.7	0.35	0.27	-22.9%	0.39	11.4%	[12]
Chloroform	Tetrahydrofuran	337.3	0.37	0.29	-21.6%	0.41	10.8%	[12]
Chloroform	Toluene	293.2	0.91	0.74	-18.7%	0.73	-19.8%	[30]
Chloroform	Toluene	293.2	0.67	0.74	10.4%	0.73	9.0%	[10]
Chloroform	Toluene	303.2	0.87	0.75	-13.8%	0.76	-12.6%	[30]
Chloroform	Toluene	313.2	0.83	0.77	-7.2%	0.78	-6.0%	[30]
Chloroform	Toluene	318.2	0.78	0.78	0.1%	0.79	1.4%	233
Chloroform	Tributyl Phosphate	298.2	0.08	0.07	-12.5%	M.G.	N.A.	[20]
Chloroform	Tributyl Phosphate	298.2	0.08	0.07	-12.5%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	298.6	0.09	0.07	-22.2%	M.G.	N.A.	[27]
Chloroform	Tributyl Phosphate	302.9	0.10	0.07	-30.0%	M.G.	N.A.	[27]
Chloroform	Tributyl Phosphate	303.2	0.09	0.07	-22.2%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	308.2	0.09	0.08	-11.1%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	308.6	0.10	0.08	-20.0%	M.G.	N.A.	[27]
Chloroform	Tributyl Phosphate	313.2	0.10	0.08	-20.0%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	318.2	0.11	0.09	-18.2%	M.G.	N.A.	[20]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Chloroform	Tributyl Phosphate	318.2	0.10	0.09	-10.0%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	323.2	0.11	0.10	-9.1%	M.G.	N.A.	[8]
Chloroform	Tributyl Phosphate	323.7	0.12	0.10	-16.7%	M.G.	N.A.	[27]
Chloroform	Tributyl Phosphate	330.0	0.12	0.10	-16.7%	M.G.	N.A.	[27]
Chloroform	Tributyl Phosphate	333.2	0.14	0.11	-21.4%	M.G.	N.A.	[20]
Chloroform	Tributyl Phosphate	363.2	0.19	0.15	-21.1%	M.G.	N.A.	[20]
Chloroform	Trichloroethylene	328.2	1.08	1.12	3.7%	1.03	-4.6%	[9]
Chloroform	Triethylamine	283.1	0.48	0.28	-41.7%	0.15	-68.8%	113
Cumene	1-Octanol	298.2	2.66	2.94	10.5%	3.38	27.1%	[32]
Cumene	Acetonitrile	298.2	6.80	6.71	-1.3%	15.78	132.1%	[64]
Cumene	Isopropanol	298.2	7.00	6.54	-6.6%	8.08	15.4%	[64]
Cumene	Methanol	298.2	15.70	15.89	1.2%	29.39	87.2%	[64]
Cumene	N-Formylmorpholine	313.3	4.95	5.67	14.5%	M.G.	N.A.	[43]
Cumene	N-Formylmorpholine	332.7	4.54	4.84	6.6%	M.G.	N.A.	[43]
Cumene	N-Formylmorpholine	352.5	4.44	4.19	-5.6%	M.G.	N.A.	[43]
Cumene	N-Formylmorpholine	373.4	4.29	3.68	-14.2%	M.G.	N.A.	[43]
Cumene	Tetrahydrofuran	298.2	0.88	0.93	5.7%	0.98	11.4%	[64]
Cycloheptane	1-Propanol	308.2	6.16	7.46	21.1%	7.35	19.3%	[47]
Cycloheptane	Dimethyl Sulfoxide	282.2	64.00	78.00	21.9%	M.P.	N.A.	[40]
Cycloheptane	Isopropanol	308.2	6.77	8.61	27.2%	6.08	-10.2%	[47]
Cycloheptane	N,N-Dimethylformamide	283.2	18.30	17.68	-3.4%	21.81	19.2%	[40]
Cycloheptane	Phenol	328.2	8.85	9.73	9.9%	6.77	-23.5%	[14]
Cycloheptane	Phenol	343.2	7.89	8.88	12.5%	6.30	-20.2%	[14]
Cycloheptane	Phenol	358.2	7.42	8.07	8.8%	5.94	-19.9%	[14]
Cycloheptane	Phenol	373.2	7.28	7.33	0.7%	5.67	-22.1%	[14]
Cycloheptane	Sulfolane	303.2	41.00	35.61	-13.1%	M.G.	N.A.	[44]
Cycloheptane	Sulfolane	313.2	35.70	29.16	-18.3%	M.G.	N.A.	[44]
Cyclohexane	1,2-Dichloroethane	293.2	3.94	3.46	-12.2%	3.30	-16.2%	[10]
Cyclohexane	1,2-Dichloroethane	298.2	4.14	3.34	-19.3%	3.17	-23.4%	120
Cyclohexane	1,2-Dichloroethane	298.2	3.82	3.34	-12.6%	3.17	-17.0%	[50]
Cyclohexane	1,4-Dioxane	298.2	4.96	3.37	-32.1%	4.26	-14.1%	[50]
Cyclohexane	1,5-Dimethyl-2-Pyrrolidinone	298.2	5.15	5.27	2.3%	M.G.	N.A.	[29]
Cyclohexane	1,5-Dimethyl-2-Pyrrolidinone	308.2	4.98	4.86	-2.4%	M.G.	N.A.	[29]
Cyclohexane	1,5-Dimethyl-2-Pyrrolidinone	318.2	4.83	4.50	-6.8%	M.G.	N.A.	[29]
Cyclohexane	1-Butanol	293.2	4.01	4.82	20.2%	4.39	9.5%	[10]
Cyclohexane	1-Butanol	298.2	4.30	4.76	10.7%	4.33	0.7%	[50]
Cyclohexane	1-Butanol	308.2	4.05	4.62	14.1%	4.21	4.0%	[30]
Cyclohexane	1-Butanol	318.2	4.08	4.47	9.6%	4.08	0.1%	159
Cyclohexane	1-Butanol	318.2	3.82	4.47	17.0%	4.08	6.8%	[30]
Cyclohexane	1-Butanol	328.2	3.82	4.31	12.8%	3.96	3.7%	[30]
Cyclohexane	1-Butanol	349.5	3.85	3.96	2.9%	3.70	-3.9%	[17]
Cyclohexane	1-Butanol	359.9	3.70	3.80	2.7%	3.58	-3.2%	[17]
Cyclohexane	1-Butanol	370.0	3.61	3.65	1.1%	3.47	-3.9%	[17]
Cyclohexane	1-Butanol	381.0	3.48	3.49	0.3%	3.36	-3.4%	[17]
Cyclohexane	1-Butanol	389.9	3.08	3.36	9.1%	3.27	6.2%	[17]
Cyclohexane	1-Chlorobutane	293.2	1.62	1.71	5.6%	1.45	-10.5%	[10]
Cyclohexane	1-Ethylpyrrolidin-2-One	298.2	5.48	5.07	-7.5%	3.54	-35.4%	[29]
Cyclohexane	1-Ethylpyrrolidin-2-One	308.2	4.98	4.68	-6.0%	3.32	-33.3%	[29]
Cyclohexane	1-Ethylpyrrolidin-2-One	318.2	4.56	4.35	-4.6%	3.13	-31.4%	[29]
Cyclohexane	1-Hexanol	293.2	2.79	3.51	25.8%	2.97	6.5%	[28]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Cyclohexane	1-Hexanol	313.2	2.51	3.32	32.3%	2.83	12.7%	[28]
Cyclohexane	1-Hexanol	333.2	2.31	3.11	34.6%	2.69	16.5%	[28]
Cyclohexane	1-Hexene	298.2	1.21	1.10	-9.1%	1.21	0.0%	[50]
Cyclohexane	1-Octanol	293.4	2.18	2.58	18.3%	2.31	6.0%	[31]
Cyclohexane	1-Octanol	298.2	2.24	2.53	12.9%	2.29	2.2%	[50]
Cyclohexane	1-Octanol	298.2	2.34	2.53	8.1%	2.29	-2.1%	[4]
Cyclohexane	1-Octanol	303.5	2.17	2.48	14.3%	2.26	4.1%	[31]
Cyclohexane	1-Octanol	313.6	2.02	2.39	18.3%	2.21	9.4%	[31]
Cyclohexane	1-Octanol	323.4	1.98	2.31	16.7%	2.16	9.1%	[31]
Cyclohexane	1-Octene	298.2	1.04	1.03	-1.0%	1.14	9.6%	[50]
Cyclohexane	1-Pentanol	303.5	3.27	3.64	11.3%	3.43	4.9%	[33]
Cyclohexane	1-Pentanol	308.2	3.42	3.60	5.3%	3.39	-0.9%	[30]
Cyclohexane	1-Pentanol	313.2	3.30	3.54	7.3%	3.34	1.2%	[33]
Cyclohexane	1-Pentanol	318.2	3.51	3.49	-0.6%	3.30	-6.0%	[30]
Cyclohexane	1-Pentanol	323.5	3.19	3.43	7.5%	3.25	1.9%	[33]
Cyclohexane	1-Pentanol	328.2	3.28	3.38	3.0%	3.21	-2.1%	[30]
Cyclohexane	1-Phenyl-1-Butanone	298.1	2.71	2.69	-0.7%	2.99	10.3%	[34]
Cyclohexane	1-Propanol	298.2	5.74	5.96	3.8%	5.90	2.8%	[50]
Cyclohexane	1-Propanol	308.2	5.30	5.80	9.4%	5.70	7.5%	[47]
Cyclohexane	2,2,4-Trimethylpentane	298.2	1.06	1.27	19.8%	1.03	-2.8%	[50]
Cyclohexane	2-Heptanone	298.2	1.99	2.22	11.6%	2.14	7.5%	[50]
Cyclohexane	2-Methyl-2-Propanol	318.2	3.19	4.12	29.0%	3.25	1.8%	155
Cyclohexane	2-Nitropropane	293.2	5.70	6.69	17.4%	5.72	0.4%	[10]
Cyclohexane	2-Pentanone	298.2	2.79	2.95	5.7%	2.95	5.7%	[50]
Cyclohexane	2-Pyrrolidone	303.2	24.54	22.66	-7.7%	M.G.	N.A.	[35]
Cyclohexane	2-Pyrrolidone	313.2	22.56	19.51	-13.5%	M.G.	N.A.	[35]
Cyclohexane	2-Pyrrolidone	323.2	20.82	16.96	-18.5%	M.G.	N.A.	[35]
Cyclohexane	2-Pyrrolidone	333.2	19.40	14.87	-23.4%	M.G.	N.A.	[35]
Cyclohexane	Acetic Acid	298.2	14.64	12.50	-14.6%	13.44	-8.2%	[50]
Cyclohexane	Acetone	298.2	6.52	7.01	7.5%	5.12	-21.5%	[50]
Cyclohexane	Acetone	308.2	5.77	6.39	10.7%	4.73	-18.0%	[75]
Cyclohexane	Acetone	323.2	5.49	5.63	2.6%	4.21	-23.3%	266
Cyclohexane	Acetonitrile	298.2	19.10	24.71	29.4%	24.43	27.9%	[36]
Cyclohexane	Acetonitrile	298.2	22.30	24.71	10.8%	24.43	9.6%	[50]
Cyclohexane	Acetophenone	293.2	4.40	4.37	-0.7%	6.84	55.5%	[10]
Cyclohexane	Acetophenone	298.2	4.60	4.19	-8.9%	6.59	43.3%	[50]
Cyclohexane	Alpha-Pinene	353.2	1.01	0.96	-5.0%	1.25	23.8%	[22]
Cyclohexane	Alpha-Pinene	373.2	1.08	0.96	-11.1%	1.24	14.8%	[22]
Cyclohexane	Aniline	293.2	12.99	12.24	-5.8%	13.40	3.2%	[37]
Cyclohexane	Aniline	293.2	13.60	12.24	-10.0%	13.40	-1.5%	[10]
Cyclohexane	Anisole	293.2	3.00	2.76	-8.0%	2.62	-12.7%	[5]
Cyclohexane	Anisole	293.2	3.10	2.76	-11.0%	2.62	-15.5%	[10]
Cyclohexane	Anisole	298.2	2.83	2.69	-4.9%	2.51	-11.3%	[50]
Cyclohexane	Anisole	343.2	2.04	2.18	6.8%	1.80	-11.8%	53
Cyclohexane	Anisole	353.2	1.97	2.10	6.5%	1.69	-14.3%	53
Cyclohexane	Benzene	293.2	1.74	1.73	-0.6%	1.78	2.3%	[58]
Cyclohexane	Benzene	293.2	1.69	1.73	2.4%	1.78	5.3%	[10]
Cyclohexane	Benzene	298.2	1.75	1.71	-2.3%	1.74	-0.6%	[50]
Cyclohexane	Benzene	314.6	1.61	1.62	0.6%	1.63	1.2%	[12]
Cyclohexane	Benzene	335.2	1.52	1.54	1.3%	1.52	0.0%	[12]
Cyclohexane	Benzene	350.6	1.45	1.48	2.1%	1.46	0.7%	[12]
Cyclohexane	Benzonitrile	293.2	4.92	5.38	9.3%	M.G.	N.A.	[10]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Cyclohexane	Benzonitrile	298.2	4.83	5.15	6.6%	M.G.	N.A.	[50]
Cyclohexane	Benzyl Acetate	298.2	3.45	3.51	1.7%	3.22	-6.7%	[10]
Cyclohexane	Benzyl Alcohol	298.2	7.96	7.42	-6.8%	9.06	13.8%	[50]
Cyclohexane	Benzyl Alcohol	298.2	7.72	7.42	-3.9%	9.06	17.4%	[67]
Cyclohexane	Butyl Acetate	298.2	1.96	2.06	5.1%	2.47	26.0%	[50]
Cyclohexane	Butyl Ether	293.2	0.95	1.18	24.2%	1.06	11.6%	[5]
Cyclohexane	Butyronitrile	298.2	5.46	5.66	3.7%	6.04	10.6%	[50]
Cyclohexane	Carbon Disulfide	298.2	1.63	1.28	-21.5%	1.67	2.5%	[50]
Cyclohexane	Carbon Tetrachloride	293.2	1.12	1.20	7.1%	1.09	-2.7%	[10]
Cyclohexane	Carbon Tetrachloride	298.2	1.10	1.19	8.2%	1.09	-0.9%	[50]
Cyclohexane	Carbon Tetrachloride	317.9	1.11	1.16	4.5%	1.08	-2.7%	[12]
Cyclohexane	Carbon Tetrachloride	330.4	1.10	1.15	4.5%	1.07	-2.7%	[12]
Cyclohexane	Carbon Tetrachloride	341.2	1.09	1.14	4.6%	1.06	-2.8%	[12]
Cyclohexane	Carbon Tetrachloride	343.2	1.10	1.14	4.1%	1.06	-3.2%	315
Cyclohexane	Carbon Tetrachloride	346.5	1.10	1.14	3.6%	1.06	-3.6%	[12]
Cyclohexane	Chlorobenzene	298.2	1.81	1.71	-5.5%	1.88	3.9%	[50]
Cyclohexane	Chlorobenzene	348.2	1.54	1.51	-2.1%	1.72	11.6%	56
Cyclohexane	Chloroform	298.2	1.66	2.05	23.5%	1.57	-5.4%	[50]
Cyclohexane	Cyclohexane	298.2	1.08	1.00	-7.4%	1.00	-7.4%	[50]
Cyclohexane	Cyclohexanone	293.2	3.08	3.44	11.7%	2.52	-18.2%	[10]
Cyclohexane	Cyclohexanone	298.2	3.00	3.34	11.3%	2.47	-17.7%	[50]
Cyclohexane	Dichloromethane	298.2	2.91	2.96	1.7%	3.16	8.6%	[50]
Cyclohexane	Diethyl Phthalate	303.2	3.24	3.22	-0.6%	M.G.	N.A.	[39]
Cyclohexane	Diethyl Phthalate	313.2	3.04	3.01	-1.0%	M.G.	N.A.	[39]
Cyclohexane	Diethyl Phthalate	323.2	2.90	2.83	-2.4%	M.G.	N.A.	[39]
Cyclohexane	Diethyl Phthalate	333.2	2.76	2.67	-3.3%	M.G.	N.A.	[39]
Cyclohexane	Diisopropyl Ether	313.2	0.95	1.33	40.0%	1.07	12.6%	[56]
Cyclohexane	Diisopropyl Ether	333.2	0.92	1.29	40.2%	1.05	14.1%	[56]
Cyclohexane	Dimethyl Carbonate	283.2	9.40	5.52	-41.3%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	293.2	8.13	5.05	-37.9%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	313.2	6.31	4.32	-31.6%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	323.2	5.65	4.03	-28.7%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	333.2	5.10	3.78	-25.8%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	343.2	4.65	3.57	-23.2%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	363.2	3.91	3.21	-17.9%	M.G.	N.A.	240
Cyclohexane	Dimethyl Carbonate	373.2	3.62	3.06	-15.5%	M.G.	N.A.	240
Cyclohexane	Dimethyl Sulfoxide	283.2	46.00	48.45	5.3%	M.P.	N.A.	[40]
Cyclohexane	Dimethyl Sulfoxide	298.2	35.47	34.16	-3.7%	M.P.	N.A.	[50]
Cyclohexane	Dimethyl Sulfoxide	313.2	35.30	25.22	-28.6%	M.P.	N.A.	[68]
Cyclohexane	Epsilon-Caprolactone	303.2	7.87	8.02	1.9%	M.G.	N.A.	[41]
Cyclohexane	Epsilon-Caprolactone	318.2	7.38	6.84	-7.3%	M.G.	N.A.	[41]
Cyclohexane	Epsilon-Caprolactone	333.2	6.74	5.95	-11.7%	M.G.	N.A.	[41]
Cyclohexane	Ethanol	297.5	10.40	11.01	5.9%	9.56	-8.1%	[48]
Cyclohexane	Ethanol	297.5	11.30	11.01	-2.6%	9.56	-15.4%	[48]
Cyclohexane	Ethanol	298.2	9.24	10.99	18.9%	9.53	3.1%	[50]
Cyclohexane	Ethanol	313.2	8.68	10.33	19.0%	8.85	2.0%	[75]
Cyclohexane	Ethanol	318.6	9.40	10.06	7.0%	8.60	-8.5%	[48]
Cyclohexane	Ethanol	318.7	9.10	10.05	10.4%	8.59	-5.6%	[48]
Cyclohexane	Ethanol	336.4	8.20	9.12	11.2%	7.79	-5.0%	[48]
Cyclohexane	Ethanol	353.2	7.60	8.23	8.3%	7.09	-6.7%	[48]
Cyclohexane	Ethyl Acetate	293.2	3.24	3.53	9.0%	3.46	6.8%	[10]
Cyclohexane	Ethyl Acetate	298.2	3.37	3.42	1.5%	3.33	-1.2%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Cyclohexane	Ethyl Acetate	303.2	3.22	3.32	3.1%	3.21	-0.3%	[75]
Cyclohexane	Ethyl Acetate	313.2	2.82	3.15	11.7%	3.00	6.4%	[19]
Cyclohexane	Ethyl Acetate	328.2	2.55	2.92	14.6%	2.72	6.7%	230
Cyclohexane	Ethyl Acetate	333.2	2.56	2.85	11.3%	2.63	2.7%	[19]
Cyclohexane	Ethyl Benzoate	313.2	2.21	2.14	-3.2%	M.G.	N.A.	[41]
Cyclohexane	Ethyl Benzoate	323.2	2.14	2.06	-3.7%	M.G.	N.A.	[41]
Cyclohexane	Ethyl Benzoate	333.2	2.08	1.99	-4.3%	M.G.	N.A.	[41]
Cyclohexane	Ethyl Benzoate	343.2	2.01	1.92	-4.5%	M.G.	N.A.	[41]
Cyclohexane	Glutaronitrile	303.2	35.80	37.55	4.9%	M.G.	N.A.	[39]
Cyclohexane	Glutaronitrile	313.2	31.60	30.95	-2.1%	M.G.	N.A.	[39]
Cyclohexane	Glutaronitrile	323.2	28.90	25.91	-10.3%	M.G.	N.A.	[39]
Cyclohexane	Glutaronitrile	333.2	26.40	21.99	-16.7%	M.G.	N.A.	[39]
Cyclohexane	Isopropanol	298.2	5.97	6.56	9.9%	5.02	-15.9%	[50]
Cyclohexane	Isopropanol	308.2	5.60	6.33	13.0%	4.86	-13.2%	[47]
Cyclohexane	Isopropanol	313.2	5.97	6.21	4.0%	4.77	-20.1%	[21]
Cyclohexane	Isopropanol	313.2	5.15	6.21	20.6%	4.77	-7.4%	[17]
Cyclohexane	Isopropanol	320.9	5.07	6.02	18.7%	4.63	-8.7%	[17]
Cyclohexane	Isopropanol	323.2	5.17	5.96	15.2%	4.59	-11.2%	228
Cyclohexane	Isopropanol	331.7	4.74	5.74	21.1%	4.45	-6.1%	[17]
Cyclohexane	Isopropanol	333.2	4.92	5.70	15.8%	4.42	-10.2%	228
Cyclohexane	Isopropanol	333.2	5.35	5.70	6.5%	4.42	-17.4%	[21]
Cyclohexane	Isopropanol	343.3	4.73	5.44	15.0%	4.25	-10.1%	[17]
Cyclohexane	Isopropanol	354.9	4.55	5.14	13.0%	4.07	-10.5%	[17]
Cyclohexane	Methanol	298.2	22.55	24.02	6.5%	21.36	-5.3%	[50]
Cyclohexane	Methanol	307.4	20.48	22.81	11.4%	20.40	-0.4%	[17]
Cyclohexane	Methanol	308.2	18.90	22.70	20.1%	20.32	7.5%	[76]
Cyclohexane	Methanol	317.2	19.48	21.35	9.6%	19.42	-0.3%	[17]
Cyclohexane	Methanol	318.2	17.40	21.20	21.8%	19.32	11.0%	[76]
Cyclohexane	Methanol	327.5	17.56	19.74	12.4%	18.43	5.0%	[17]
Cyclohexane	Methanol	333.2	16.60	18.83	13.4%	17.90	7.8%	[76]
Cyclohexane	Methanol	337.3	16.16	18.19	12.6%	17.52	8.4%	[17]
Cyclohexane	Methyl Acetate	298.2	5.28	6.17	16.9%	5.29	0.2%	[50]
Cyclohexane	Methyl Ethyl Ketone	298.2	3.78	3.98	5.3%	3.72	-1.6%	[50]
Cyclohexane	Methyl Ethyl Ketone	323.2	3.16	3.42	8.2%	3.20	1.3%	335
Cyclohexane	Methyl Isobutyl Ketone	293.2	2.01	2.41	19.9%	2.53	25.9%	[5]
Cyclohexane	Methyl Tert-Butyl Ether	313.2	1.21	1.40	15.7%	1.26	4.1%	[56]
Cyclohexane	Methyl Tert-Butyl Ether	333.2	1.07	1.35	26.2%	1.20	12.1%	[56]
Cyclohexane	N,N-Dibutylformamide	302.8	2.13	2.35	10.5%	2.23	4.9%	[13]
Cyclohexane	N,N-Dibutylformamide	318.3	1.97	2.18	10.4%	2.10	6.4%	[13]
Cyclohexane	N,N-Dibutylformamide	332.4	1.89	2.05	8.5%	1.99	5.3%	[13]
Cyclohexane	N,N-Diethylacetamide	303.2	3.74	3.95	5.6%	2.19	-41.4%	[39]
Cyclohexane	N,N-Diethylacetamide	313.2	3.53	3.69	4.5%	2.12	-39.9%	[39]
Cyclohexane	N,N-Diethylacetamide	323.2	3.33	3.47	4.2%	2.06	-38.1%	[39]
Cyclohexane	N,N-Diethylacetamide	333.2	3.16	3.28	3.8%	2.00	-36.7%	[39]
Cyclohexane	N,N-Dimethylacetamide	303.6	6.54	6.82	4.2%	6.88	5.2%	[13]
Cyclohexane	N,N-Dimethylacetamide	317.6	6.20	5.96	-3.9%	6.19	-0.2%	[13]
Cyclohexane	N,N-Dimethylacetamide	333.4	5.90	5.22	-11.6%	5.54	-6.1%	[13]
Cyclohexane	N,N-Dimethylformamide	283.2	15.60	12.98	-16.8%	14.89	-4.6%	[40]
Cyclohexane	N,N-Dimethylformamide	293.2	13.10	11.29	-13.8%	12.99	-0.8%	[10]
Cyclohexane	N-Decane	298.2	0.95	0.92	-3.2%	0.99	4.2%	[50]
Cyclohexane	N-Dodecane	298.2	0.94	0.84	-10.6%	0.94	0.0%	[50]
Cyclohexane	N-Ethylacetamide	303.2	6.27	6.68	6.5%	M.G.	N.A.	[39]

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Cyclohexane	N-Ethylacetamide	313.2	6.12	6.34	3.6%	M.G.	N.A.	[39]
Cyclohexane	N-Ethylacetamide	323.2	6.02	6.01	-0.2%	M.G.	N.A.	[39]
Cyclohexane	N-Ethylacetamide	333.2	5.89	5.69	-3.4%	M.G.	N.A.	[39]
Cyclohexane	N-Formylmorpholine	313.3	16.70	16.09	-3.7%	M.G.	N.A.	[43]
Cyclohexane	N-Formylmorpholine	332.7	13.50	12.51	-7.3%	M.G.	N.A.	[43]
Cyclohexane	N-Formylmorpholine	352.5	11.70	10.01	-14.4%	M.G.	N.A.	[43]
Cyclohexane	N-Formylmorpholine	373.4	10.00	8.16	-18.4%	M.G.	N.A.	[43]
Cyclohexane	N-Heptane	293.2	0.99	1.07	8.1%	1.07	8.1%	[10]
Cyclohexane	N-Heptane	298.2	1.10	1.07	-2.7%	1.06	-3.6%	[50]
Cyclohexane	N-Hexadecane	293.2	0.82	0.72	-12.2%	0.87	6.1%	[70]
Cyclohexane	N-Hexadecane	298.1	0.79	0.72	-8.9%	0.86	8.9%	[77]
Cyclohexane	N-Hexadecane	298.2	0.81	0.72	-11.1%	0.86	6.2%	[70]
Cyclohexane	N-Hexadecane	298.2	0.80	0.72	-10.0%	0.86	7.5%	[50]
Cyclohexane	N-Hexadecane	298.2	0.82	0.72	-11.9%	0.86	5.3%	[6]
Cyclohexane	N-Hexadecane	298.2	0.79	0.72	-8.9%	0.86	8.9%	[78]
Cyclohexane	N-Hexadecane	303.2	0.81	0.72	-11.1%	0.86	6.2%	[70]
Cyclohexane	N-Hexadecane	313.2	0.80	0.72	-10.0%	0.85	6.2%	[70]
Cyclohexane	N-Hexadecane	313.2	0.76	0.72	-5.3%	0.85	11.8%	[78]
Cyclohexane	N-Hexadecane	323.2	0.79	0.72	-8.9%	0.84	6.3%	[70]
Cyclohexane	N-Hexadecane	323.2	0.76	0.72	-5.3%	0.84	10.5%	[78]
Cyclohexane	N-Hexadecane	333.2	0.78	0.72	-7.7%	0.84	7.7%	[70]
Cyclohexane	N-Hexadecane	333.2	0.74	0.72	-2.7%	0.84	13.5%	[78]
Cyclohexane	N-Hexane	298.2	1.14	1.14	0.0%	1.10	-3.5%	[50]
Cyclohexane	N-Hexane	301.0	1.09	1.14	4.6%	1.09	0.0%	[12]
Cyclohexane	N-Hexane	315.3	1.09	1.13	3.7%	1.08	-0.9%	[12]
Cyclohexane	N-Hexane	332.0	1.07	1.13	5.6%	1.06	-0.9%	[12]
Cyclohexane	N-Hexane	340.3	1.06	1.12	5.7%	1.06	0.0%	[12]
Cyclohexane	N-Hexane	341.0	1.05	1.12	6.7%	1.06	1.0%	[17]
Cyclohexane	Nitrobenzene	293.2	5.79	5.44	-6.0%	5.87	1.4%	[10]
Cyclohexane	Nitrobenzene	298.2	6.12	5.19	-15.2%	5.67	-7.4%	[50]
Cyclohexane	Nitroethane	293.2	9.61	11.03	14.8%	9.47	-1.5%	[10]
Cyclohexane	Nitromethane	293.2	36.80	40.43	9.9%	48.33	31.3%	[10]
Cyclohexane	Nitromethane	298.2	36.68	36.16	-1.4%	45.10	23.0%	[50]
Cyclohexane	N-Methyl-2-Pyrrolidone	298.2	8.31	6.99	-15.9%	8.07	-2.9%	[50]
Cyclohexane	N-Methyl-2-Pyrrolidone	323.4	8.18	5.53	-32.4%	6.58	-19.6%	[43]
Cyclohexane	N-Methyl-2-Pyrrolidone	333.2	7.66	5.11	-33.3%	6.10	-20.4%	[43]
Cyclohexane	N-Methyl-2-Pyrrolidone	333.3	4.33	5.11	18.1%	6.10	40.9%	238
Cyclohexane	N-Methyl-2-Pyrrolidone	343.4	7.34	4.74	-35.4%	5.66	-22.9%	[43]
Cyclohexane	N-Methyl-2-Pyrrolidone	354.2	3.84	4.41	14.7%	5.23	36.1%	238
Cyclohexane	N-Methylacetamide	318.4	9.31	9.11	-2.2%	8.73	-6.2%	[13]
Cyclohexane	N-Methylacetamide	333.2	8.84	8.28	-6.3%	8.30	-6.1%	[13]
Cyclohexane	N-Methylformamide	298.2	23.32	25.97	11.4%	M.P.	N.A.	[50]
Cyclohexane	N-Methylformamide	303.2	23.88	24.68	3.4%	M.P.	N.A.	[35]
Cyclohexane	N-Methylformamide	313.2	22.51	22.26	-1.1%	M.P.	N.A.	[35]
Cyclohexane	N-Methylformamide	323.2	21.23	20.06	-5.5%	M.P.	N.A.	[35]
Cyclohexane	N-Methylformamide	333.2	20.05	18.09	-9.8%	M.P.	N.A.	[35]
Cyclohexane	N-Nonane	298.2	0.99	0.96	-3.0%	1.01	2.0%	[50]
Cyclohexane	N-Octane	298.2	1.05	1.01	-3.8%	1.03	-1.9%	[50]
Cyclohexane	N-Pentane	298.2	1.30	1.27	-2.3%	1.15	-11.5%	[50]
Cyclohexane	Phenol	323.2	7.20	7.96	10.6%	5.46	-24.2%	[10]
Cyclohexane	Phenol	328.2	8.48	7.75	-8.6%	5.33	-37.1%	[14]
Cyclohexane	Phenol	343.2	7.59	7.15	-5.8%	5.01	-34.0%	[14]

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Cyclohexane	Phenol	358.2	7.10	6.57	-7.5%	4.76	-33.0%	[14]
Cyclohexane	Phenol	373.2	6.97	6.03	-13.5%	4.58	-34.3%	[14]
Cyclohexane	Propionitrile	293.2	8.40	10.32	22.9%	7.95	-5.4%	[10]
Cyclohexane	Propionitrile	298.2	9.08	9.66	6.4%	7.70	-15.2%	[50]
Cyclohexane	Propionitrile	336.7	6.00	6.34	5.7%	6.19	3.2%	[12]
Cyclohexane	Propionitrile	356.3	5.22	5.36	2.7%	5.65	8.2%	[12]
Cyclohexane	P-Xylene	293.2	1.35	1.34	-0.7%	1.47	8.9%	[10]
Cyclohexane	P-Xylene	298.2	1.42	1.32	-7.0%	1.45	2.1%	[50]
Cyclohexane	Pyridine	293.2	4.48	4.59	2.4%	5.12	14.2%	157
Cyclohexane	Pyridine	298.2	4.27	4.41	3.2%	5.03	17.7%	157
Cyclohexane	Pyridine	298.2	4.45	4.41	-0.9%	5.03	13.0%	[50]
Cyclohexane	Pyridine	303.2	4.11	4.24	3.2%	4.93	20.0%	157
Cyclohexane	Pyridine	308.2	3.94	4.08	3.7%	4.85	23.2%	157
Cyclohexane	Pyridine	313.2	3.77	3.93	4.3%	4.76	26.3%	157
Cyclohexane	Quinoline	293.2	5.68	4.70	-17.3%	M.G.	N.A.	[37]
Cyclohexane	Quinoline	298.2	4.35	4.52	3.9%	M.G.	N.A.	[10]
Cyclohexane	Squalane	298.2	0.53	0.61	15.1%	0.67	26.4%	[50]
Cyclohexane	Sulfolane	303.6	28.10	24.20	-13.9%	M.G.	N.A.	[13]
Cyclohexane	Sulfolane	317.9	21.20	18.86	-11.0%	M.G.	N.A.	[13]
Cyclohexane	Sulfolane	333.2	16.06	14.94	-7.0%	M.G.	N.A.	[13]
Cyclohexane	Tetraethylene Glycol DME	304.6	2.75	2.83	3.1%	1.79	-34.8%	[7]
Cyclohexane	Tetraethylene Glycol DME	323.2	2.49	2.55	2.2%	1.56	-37.4%	[7]
Cyclohexane	Tetraethylene Glycol DME	343.2	2.22	2.32	4.4%	1.36	-38.8%	[7]
Cyclohexane	Tetrahydrofuran	298.2	2.14	2.01	-5.9%	1.79	-16.2%	307
Cyclohexane	Tetrahydrofuran	298.2	1.87	2.01	7.5%	1.79	-4.3%	[50]
Cyclohexane	Tetrahydrofuran	313.2	1.76	1.90	8.0%	1.70	-3.4%	[19]
Cyclohexane	Tetrahydrofuran	327.7	1.69	1.82	7.7%	1.62	-4.1%	[12]
Cyclohexane	Tetrahydrofuran	333.2	1.65	1.79	8.5%	1.59	-3.6%	[19]
Cyclohexane	Tetrahydrofuran	337.3	1.59	1.76	10.7%	1.57	-1.3%	[12]
Cyclohexane	Toluene	293.2	1.59	1.50	-5.7%	1.60	0.6%	[10]
Cyclohexane	Toluene	298.2	1.56	1.49	-4.5%	1.57	0.6%	[50]
Cyclohexane	Tributyl Phosphate	298.2	1.56	1.65	5.8%	M.G.	N.A.	[20]
Cyclohexane	Tributyl Phosphate	298.6	1.51	1.65	9.3%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	302.9	1.48	1.62	9.5%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	308.6	1.46	1.58	8.2%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	313.1	1.45	1.55	6.9%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	318.2	1.36	1.52	11.8%	M.G.	N.A.	[20]
Cyclohexane	Tributyl Phosphate	323.7	1.34	1.48	10.4%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	330.0	1.28	1.45	13.3%	M.G.	N.A.	[27]
Cyclohexane	Tributyl Phosphate	333.2	1.19	1.43	20.2%	M.G.	N.A.	[20]
Cyclohexane	Triethylamine	298.2	1.22	1.27	4.1%	M.P.	N.A.	[50]
Cyclohexanone	N-Hexane	298.0	7.10	5.55	-21.8%	4.68	-34.1%	[12]
Cyclohexanone	N-Hexane	315.1	5.30	4.71	-11.1%	4.12	-22.3%	[12]
Cyclohexanone	N-Hexane	331.7	4.70	4.10	-12.8%	3.70	-21.3%	[12]
Cyclooctane	Dimethyl Sulfoxide	283.2	77.00	117.89	53.1%	M.P.	N.A.	[40]
Cyclooctane	N,N-Dimethylformamide	283.2	25.70	23.76	-7.5%	31.71	23.4%	[40]
Cyclooctane	Sulfolane	303.2	51.00	51.92	1.8%	M.G.	N.A.	[44]
Cyclooctane	Sulfolane	313.2	43.60	41.59	-4.6%	M.G.	N.A.	[44]
Cyclopentane	1-Propanol	308.2	4.40	4.66	5.9%	4.35	-1.1%	[47]
Cyclopentane	2-Pyrrolidone	303.2	17.18	15.58	-9.3%	M.G.	N.A.	[35]
Cyclopentane	2-Pyrrolidone	313.2	15.99	13.68	-14.4%	M.G.	N.A.	[35]
Cyclopentane	2-Pyrrolidone	323.2	15.10	12.11	-19.8%	M.G.	N.A.	[35]

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Cyclopentane	2-Pyrrolidone	333.2	14.11	10.80	-23.5%	M.G.	N.A.	[35]
Cyclopentane	Acetone	308.2	4.45	4.99	12.1%	3.81	-14.4%	[75]
Cyclopentane	Aniline	293.2	9.18	8.91	-2.9%	8.89	-3.2%	[37]
Cyclopentane	Benzyl Alcohol	298.2	5.88	5.69	-3.2%	6.26	6.5%	[67]
Cyclopentane	Ethanol	313.2	6.80	7.86	15.6%	6.40	-5.9%	[75]
Cyclopentane	Ethyl Acetate	303.2	2.73	2.76	1.1%	2.75	0.7%	[75]
Cyclopentane	Ethyl Benzoate	313.2	1.89	1.86	-1.6%	M.G.	N.A.	[41]
Cyclopentane	Ethyl Benzoate	323.2	1.86	1.79	-3.8%	M.G.	N.A.	[41]
Cyclopentane	Ethyl Benzoate	333.2	1.82	1.74	-4.4%	M.G.	N.A.	[41]
Cyclopentane	Ethyl Benzoate	343.2	1.79	1.69	-5.6%	M.G.	N.A.	[41]
Cyclopentane	Isopropanol	308.2	4.59	4.95	7.8%	3.83	-16.6%	[47]
Cyclopentane	Methanol	288.2	16.20	17.68	9.1%	14.80	-8.6%	[79]
Cyclopentane	Methyl Tert-Butyl Ether	288.2	1.69	1.33	-21.3%	1.28	-24.3%	[79]
Cyclopentane	Methyl Tert-Butyl Ether	313.2	1.16	1.28	10.3%	1.22	5.2%	[56]
Cyclopentane	Methyl Tert-Butyl Ether	323.2	1.10	1.27	15.5%	1.20	9.1%	[56]
Cyclopentane	N-Formylmorpholine	313.3	11.70	11.11	-5.0%	M.G.	N.A.	[43]
Cyclopentane	N-Formylmorpholine	332.7	9.92	8.93	-10.0%	M.G.	N.A.	[43]
Cyclopentane	N-Formylmorpholine	352.5	8.76	7.36	-16.0%	M.G.	N.A.	[43]
Cyclopentane	N-Formylmorpholine	373.4	7.60	6.17	-18.8%	M.G.	N.A.	[43]
Cyclopentane	N-Hexadecane	293.1	0.77	0.66	-14.3%	0.81	5.2%	[80]
Cyclopentane	N-Hexadecane	298.1	0.75	0.66	-12.0%	0.80	6.7%	[80]
Cyclopentane	N-Hexadecane	303.1	0.75	0.66	-12.0%	0.80	6.7%	[80]
Cyclopentane	N-Methyl-2-Pyrrolidone	323.4	6.41	4.51	-29.6%	4.60	-28.2%	[43]
Cyclopentane	N-Methyl-2-Pyrrolidone	333.2	6.07	4.21	-30.6%	4.32	-28.8%	[43]
Cyclopentane	N-Methyl-2-Pyrrolidone	343.4	5.84	3.94	-32.5%	4.05	-30.7%	[43]
Cyclopentane	Quinoline	293.2	4.04	3.78	-6.4%	M.G.	N.A.	[37]
Dichloromethane	1,2-Dichloroethane	293.2	1.02	0.99	-2.9%	1.02	0.0%	[10]
Dichloromethane	1,2-Dichloroethane	328.2	1.05	0.99	-5.7%	1.02	-2.9%	[1]
Dichloromethane	1,4-Dioxane	303.2	0.53	0.52	-1.1%	0.35	-33.4%	199
Dichloromethane	1,5-Dimethyl-2-Pyrrolidinone	298.2	0.24	0.24	-1.2%	M.G.	N.A.	[29]
Dichloromethane	1,5-Dimethyl-2-Pyrrolidinone	308.2	0.28	0.27	-2.2%	M.G.	N.A.	[29]
Dichloromethane	1,5-Dimethyl-2-Pyrrolidinone	318.2	0.31	0.29	-5.2%	M.G.	N.A.	[29]
Dichloromethane	1-Butanol	293.2	1.86	2.08	11.8%	2.00	7.5%	[10]
Dichloromethane	1-Butanol	308.2	1.97	2.01	2.0%	1.97	0.0%	[30]
Dichloromethane	1-Butanol	318.2	1.94	1.96	1.0%	1.95	0.5%	[30]
Dichloromethane	1-Butanol	328.2	1.92	1.91	-0.5%	1.94	1.0%	[30]
Dichloromethane	1-Chlorobutane	293.2	1.02	1.09	6.9%	1.07	4.9%	[10]
Dichloromethane	1-Ethylpyrrolidin-2-One	298.2	0.27	0.27	0.0%	M.P.	N.A.	[29]
Dichloromethane	1-Ethylpyrrolidin-2-One	308.2	0.30	0.30	0.7%	M.P.	N.A.	[29]
Dichloromethane	1-Ethylpyrrolidin-2-One	318.2	0.34	0.32	-6.2%	M.P.	N.A.	[29]
Dichloromethane	1-Octanol	293.2	1.56	1.41	-9.6%	1.74	11.5%	[10]
Dichloromethane	1-Octanol	298.2	1.57	1.39	-11.5%	1.71	8.9%	[2]
Dichloromethane	1-Octanol	298.2	1.47	1.39	-5.4%	1.71	16.3%	[3]
Dichloromethane	1-Octanol	298.2	1.57	1.39	-11.5%	1.71	8.9%	[4]
Dichloromethane	1-Octanol	308.2	1.58	1.35	-14.6%	1.66	5.1%	[2]
Dichloromethane	1-Octanol	323.2	1.45	1.29	-11.0%	1.59	9.7%	[2]
Dichloromethane	1-Pentanol	303.5	1.82	1.94	6.6%	1.89	3.8%	[33]
Dichloromethane	1-Pentanol	308.2	2.09	1.92	-8.1%	1.88	-10.0%	[30]
Dichloromethane	1-Pentanol	313.2	1.76	1.89	7.4%	1.86	5.7%	[33]
Dichloromethane	1-Pentanol	318.2	1.84	1.87	1.6%	1.85	0.5%	[30]

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Dichloromethane	1-Pentanol	323.5	1.78	1.84	3.4%	1.83	2.8%	[33]
Dichloromethane	1-Pentanol	328.2	1.80	1.82	1.1%	1.82	1.1%	[30]
Dichloromethane	1-Phenyl-1-Butanone	298.1	0.65	0.60	-7.7%	0.61	-6.2%	[34]
Dichloromethane	2,2,4-Trimethylpentane	293.2	2.13	2.41	13.1%	1.90	-10.8%	[10]
Dichloromethane	2-Nitropropane	293.2	0.91	0.93	2.2%	0.98	7.7%	[10]
Dichloromethane	2-Pyrrolidone	303.2	0.82	0.97	18.1%	M.G.	N.A.	[35]
Dichloromethane	2-Pyrrolidone	313.2	0.86	0.97	12.4%	M.G.	N.A.	[35]
Dichloromethane	2-Pyrrolidone	323.2	0.91	0.96	6.0%	M.G.	N.A.	[35]
Dichloromethane	2-Pyrrolidone	333.2	0.95	0.96	0.9%	M.G.	N.A.	[35]
Dichloromethane	Acetone	298.2	0.61	0.62	0.9%	0.53	-13.8%	221
Dichloromethane	Acetone	303.2	0.58	0.63	9.5%	0.54	-6.1%	221
Dichloromethane	Acetone	348.2	0.71	0.74	4.6%	0.63	-10.9%	221
Dichloromethane	Acetone	398.2	0.79	0.82	4.4%	0.70	-10.9%	221
Dichloromethane	Acetonitrile	298.2	1.20	1.44	20.0%	1.16	-3.4%	223
Dichloromethane	Acetonitrile	348.2	1.25	1.34	7.1%	1.25	-0.1%	223
Dichloromethane	Acetonitrile	398.1	1.28	1.27	-1.0%	1.33	3.7%	223
Dichloromethane	Acetophenone	293.2	0.62	0.70	12.9%	0.70	12.9%	[10]
Dichloromethane	Aniline	293.2	1.41	1.24	-12.1%	M.P.	N.A.	[10]
Dichloromethane	Anisole	293.2	0.77	0.75	-2.6%	0.40	-48.1%	[10]
Dichloromethane	Benzene	293.2	0.91	0.96	5.5%	0.96	5.5%	[58]
Dichloromethane	Benzene	293.2	0.92	0.96	4.3%	0.96	4.3%	[10]
Dichloromethane	Benzene	298.2	0.89	0.97	9.3%	0.96	8.1%	204
Dichloromethane	Benzene	348.0	0.93	0.98	5.3%	0.98	5.3%	204
Dichloromethane	Benzonitrile	293.2	0.70	0.61	-12.9%	M.G.	N.A.	[10]
Dichloromethane	Carbon Tetrachloride	293.2	1.58	1.57	-0.6%	1.58	0.0%	[10]
Dichloromethane	Carbon Tetrachloride	328.2	1.49	1.43	-4.0%	1.45	-2.7%	[1]
Dichloromethane	Chlorobenzene	298.0	1.07	0.88	-17.6%	1.03	-3.6%	147
Dichloromethane	Chlorobenzene	348.0	1.05	0.90	-14.7%	1.02	-3.3%	147
Dichloromethane	Chlorobenzene	398.1	1.07	0.92	-14.0%	1.03	-3.7%	147
Dichloromethane	Chloroform	298.2	1.26	1.01	-19.8%	1.05	-16.7%	[30]
Dichloromethane	Chloroform	308.2	1.06	1.01	-4.7%	1.05	-0.9%	[1]
Dichloromethane	Cyclohexanone	293.2	0.39	0.44	12.8%	0.61	56.4%	[10]
Dichloromethane	Diethyl Phthalate	303.2	0.51	0.51	0.4%	M.G.	N.A.	[39]
Dichloromethane	Diethyl Phthalate	313.2	0.52	0.52	0.2%	M.G.	N.A.	[39]
Dichloromethane	Diethyl Phthalate	323.2	0.53	0.53	-0.6%	M.G.	N.A.	[39]
Dichloromethane	Diethyl Phthalate	333.2	0.54	0.54	0.2%	M.G.	N.A.	[39]
Dichloromethane	Dimethyl Sulfoxide	298.2	0.56	0.41	-27.3%	0.76	34.7%	303
Dichloromethane	Epsilon-Caprolactone	303.2	0.53	0.58	9.6%	M.G.	N.A.	[41]
Dichloromethane	Epsilon-Caprolactone	318.2	0.56	0.62	10.7%	M.G.	N.A.	[41]
Dichloromethane	Epsilon-Caprolactone	333.2	0.59	0.65	10.0%	M.G.	N.A.	[41]
Dichloromethane	Ethanol	298.2	2.50	3.00	20.0%	2.17	-13.2%	[30]
Dichloromethane	Ethyl Acetate	293.2	0.49	0.59	20.4%	0.52	6.1%	[10]
Dichloromethane	Ethyl Acetate	298.2	0.58	0.61	5.2%	0.54	-6.9%	222
Dichloromethane	Ethyl Acetate	348.2	0.65	0.70	8.3%	0.61	-5.6%	222
Dichloromethane	Ethyl Acetate	398.2	0.71	0.76	7.3%	0.60	-15.3%	222
Dichloromethane	Glutaronitrile	303.2	1.20	1.44	20.0%	M.G.	N.A.	[39]
Dichloromethane	Glutaronitrile	313.2	1.22	1.41	15.6%	M.G.	N.A.	[39]
Dichloromethane	Glutaronitrile	323.2	1.25	1.38	10.4%	M.G.	N.A.	[39]
Dichloromethane	Glutaronitrile	333.2	1.27	1.36	7.1%	M.G.	N.A.	[39]
Dichloromethane	Methanol	298.2	2.81	4.17	48.4%	2.89	2.8%	[30]
Dichloromethane	Methanol	298.2	3.26	4.16	27.6%	2.89	-11.4%	220
Dichloromethane	Methanol	348.2	3.20	3.60	12.4%	2.88	-10.0%	220

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Dichloromethane	Methanol	398.2	3.25	2.98	-8.2%	2.63	-19.0%	220
Dichloromethane	Methyl Ethyl Ketone	293.2	0.51	0.52	2.0%	0.53	3.9%	[10]
Dichloromethane	N,N-Dibutylformamide	302.8	0.32	0.29	-10.5%	0.32	-1.2%	[13]
Dichloromethane	N,N-Dibutylformamide	318.3	0.34	0.32	-6.4%	0.35	2.3%	[13]
Dichloromethane	N,N-Dibutylformamide	332.4	0.36	0.35	-3.8%	0.38	4.4%	[13]
Dichloromethane	N,N-Diethylacetamide	303.2	0.26	0.29	11.5%	0.38	46.2%	[39]
Dichloromethane	N,N-Diethylacetamide	313.2	0.28	0.31	10.3%	0.40	42.3%	[39]
Dichloromethane	N,N-Diethylacetamide	323.2	0.31	0.34	9.3%	0.43	38.3%	[39]
Dichloromethane	N,N-Diethylacetamide	333.2	0.33	0.36	9.4%	0.45	36.8%	[39]
Dichloromethane	N,N-Dimethylacetamide	303.6	0.32	0.34	5.9%	0.31	-3.4%	[13]
Dichloromethane	N,N-Dimethylacetamide	317.6	0.36	0.38	5.6%	0.35	-2.8%	[13]
Dichloromethane	N,N-Dimethylacetamide	333.0	0.40	0.42	4.2%	0.39	-3.2%	[13]
Dichloromethane	N-Ethylacetamide	303.2	0.87	1.01	16.6%	M.G.	N.A.	[39]
Dichloromethane	N-Ethylacetamide	313.2	0.91	1.00	10.5%	M.G.	N.A.	[39]
Dichloromethane	N-Ethylacetamide	323.2	0.95	1.00	4.8%	M.G.	N.A.	[39]
Dichloromethane	N-Ethylacetamide	333.2	0.99	1.00	0.8%	M.G.	N.A.	[39]
Dichloromethane	N-Heptane	293.2	2.20	2.36	7.3%	1.97	-10.5%	[10]
Dichloromethane	N-Hexadecane	298.2	1.41	1.55	9.7%	1.46	3.3%	[6]
Dichloromethane	N-Hexane	298.2	2.13	2.42	13.5%	2.01	-5.7%	331
Dichloromethane	Nitrobenzene	293.2	0.99	0.86	-13.1%	M.P.	N.A.	[10]
Dichloromethane	Nitroethane	293.2	0.92	1.05	14.1%	0.97	5.4%	[10]
Dichloromethane	Nitromethane	293.2	1.68	1.79	6.5%	1.71	1.8%	[10]
Dichloromethane	Nitromethane	298.1	1.66	1.76	6.0%	1.71	3.0%	191
Dichloromethane	Nitromethane	348.0	1.61	1.56	-3.0%	1.57	-2.3%	191
Dichloromethane	Nitromethane	398.1	1.55	1.44	-7.3%	1.22	-21.4%	191
Dichloromethane	N-Methylacetamide	303.3	1.02	1.23	20.4%	M.P.	N.A.	[13]
Dichloromethane	N-Methylacetamide	318.4	1.04	1.22	17.8%	M.P.	N.A.	[13]
Dichloromethane	N-Methylacetamide	333.2	1.05	1.21	15.1%	M.P.	N.A.	[13]
Dichloromethane	N-Methylformamide	303.2	1.48	1.87	26.1%	M.P.	N.A.	[35]
Dichloromethane	N-Methylformamide	313.2	1.54	1.84	19.9%	M.P.	N.A.	[35]
Dichloromethane	N-Methylformamide	323.2	1.59	1.81	14.2%	M.P.	N.A.	[35]
Dichloromethane	N-Methylformamide	333.2	1.63	1.78	9.1%	M.P.	N.A.	[35]
Dichloromethane	N-Octane	293.2	2.15	2.23	3.7%	1.90	-11.6%	[10]
Dichloromethane	N-Pentane	298.2	2.61	2.62	0.3%	2.08	-20.4%	146
Dichloromethane	N-Pentane	348.2	1.94	2.01	3.8%	1.73	-10.7%	146
Dichloromethane	N-Pentane	398.2	1.58	1.68	6.4%	1.44	-8.8%	146
Dichloromethane	Phenol	323.2	1.71	2.01	17.5%	M.P.	N.A.	[10]
Dichloromethane	Propionitrile	293.2	0.82	0.93	13.4%	0.78	-4.9%	[10]
Dichloromethane	P-Xylene	293.2	0.85	1.02	20.0%	0.85	0.0%	[10]
Dichloromethane	Pyridine	303.2	0.63	0.63	0.5%	0.52	-17.0%	296
Dichloromethane	Sulfolane	303.8	0.90	0.96	6.5%	M.G.	N.A.	[13]
Dichloromethane	Sulfolane	317.9	0.94	0.97	3.2%	M.G.	N.A.	[13]
Dichloromethane	Sulfolane	334.2	0.98	0.97	-1.0%	M.G.	N.A.	[13]
Dichloromethane	Tetraethylene Glycol DME	303.2	0.20	0.28	42.1%	0.11	-44.2%	[7]
Dichloromethane	Tetraethylene Glycol DME	323.2	0.25	0.31	23.5%	0.18	-28.3%	[7]
Dichloromethane	Tetraethylene Glycol DME	343.2	0.30	0.35	15.1%	0.30	-1.3%	[7]
Dichloromethane	Tetrahydrofuran	293.7	0.41	0.44	7.3%	0.48	17.1%	[12]
Dichloromethane	Tetrahydrofuran	303.2	0.35	0.47	33.9%	0.49	39.5%	299
Dichloromethane	Tetrahydrofuran	311.5	0.45	0.49	8.9%	0.50	11.1%	[12]
Dichloromethane	Tetrahydrofuran	328.4	0.48	0.53	10.4%	0.52	8.3%	[12]
Dichloromethane	Tetrahydrofuran	336.9	0.50	0.56	12.0%	0.53	6.0%	[12]
Dichloromethane	Toluene	293.2	0.83	0.99	19.3%	0.87	4.8%	[33]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Dichloromethane	Toluene	293.2	0.83	0.99	19.3%	0.87	4.8%	[33]
Dichloromethane	Toluene	293.2	0.85	0.99	16.5%	0.87	2.4%	[10]
Dichloromethane	Toluene	298.2	0.81	0.99	22.6%	0.87	7.7%	203
Dichloromethane	Toluene	303.2	0.84	0.99	17.9%	0.88	4.8%	[33]
Dichloromethane	Toluene	313.2	1.00	0.98	-2.0%	0.89	-11.0%	[33]
Dichloromethane	Toluene	347.9	0.88	0.98	11.6%	0.92	4.8%	203
Dichloromethane	Tributyl Phosphate	298.2	0.18	0.18	0.0%	M.G.	N.A.	[8]
Dichloromethane	Tributyl Phosphate	303.2	0.18	0.18	0.0%	M.G.	N.A.	[8]
Dichloromethane	Tributyl Phosphate	308.2	0.18	0.19	5.6%	M.G.	N.A.	[8]
Dichloromethane	Tributyl Phosphate	313.2	0.18	0.20	11.1%	M.G.	N.A.	[8]
Dichloromethane	Tributyl Phosphate	318.2	0.18	0.20	11.1%	M.G.	N.A.	[8]
Dichloromethane	Tributyl Phosphate	323.2	0.18	0.21	16.7%	M.G.	N.A.	[8]
Dichloromethane	Triethylamine	283.2	0.82	0.82	0.4%	0.71	-13.1%	112
Diethyl Ether	1,5-Dimethyl-2-Pyrrolidinone	298.2	2.66	2.68	0.8%	M.G.	N.A.	[29]
Diethyl Ether	1,5-Dimethyl-2-Pyrrolidinone	308.2	2.66	2.56	-3.8%	M.G.	N.A.	[29]
Diethyl Ether	1,5-Dimethyl-2-Pyrrolidinone	318.2	2.64	2.46	-6.8%	M.G.	N.A.	[29]
Diethyl Ether	1-Butanol	308.2	1.88	1.71	-9.0%	2.14	13.8%	[30]
Diethyl Ether	1-Butanol	318.2	1.81	1.70	-6.1%	2.11	16.6%	[30]
Diethyl Ether	1-Butanol	328.2	1.68	1.68	0.0%	2.09	24.4%	[30]
Diethyl Ether	1-Ethylpyrrolidin-2-One	298.2	2.86	2.75	-3.8%	M.P.	N.A.	[29]
Diethyl Ether	1-Ethylpyrrolidin-2-One	308.2	2.75	2.63	-4.4%	M.P.	N.A.	[29]
Diethyl Ether	1-Ethylpyrrolidin-2-One	318.2	2.66	2.53	-4.9%	M.P.	N.A.	[29]
Diethyl Ether	1-Octanol	298.2	1.42	1.34	-5.6%	1.51	6.3%	[3]
Diethyl Ether	1-Pentanol	303.5	1.67	1.58	-5.4%	1.91	14.4%	[33]
Diethyl Ether	1-Pentanol	308.2	1.75	1.57	-10.3%	1.90	8.6%	[30]
Diethyl Ether	1-Pentanol	313.2	1.66	1.56	-6.0%	1.88	13.3%	[33]
Diethyl Ether	1-Pentanol	318.2	1.95	1.55	-20.5%	1.87	-4.1%	[30]
Diethyl Ether	1-Pentanol	323.5	1.67	1.54	-7.8%	1.86	11.4%	[33]
Diethyl Ether	1-Pentanol	328.2	1.59	1.53	-3.8%	1.85	16.4%	[30]
Diethyl Ether	1-Phenyl-1-Butanone	298.1	1.62	1.45	-10.5%	1.68	3.7%	[34]
Diethyl Ether	2-Pyrrolidone	303.2	7.47	8.65	15.8%	M.G.	N.A.	[35]
Diethyl Ether	2-Pyrrolidone	313.2	7.23	7.85	8.6%	M.G.	N.A.	[35]
Diethyl Ether	2-Pyrrolidone	323.2	7.02	7.17	2.1%	M.G.	N.A.	[35]
Diethyl Ether	2-Pyrrolidone	333.2	6.85	6.57	-4.1%	M.G.	N.A.	[35]
Diethyl Ether	Acetone	298.1	1.94	1.88	-3.1%	2.16	11.3%	149
Diethyl Ether	Acetone	338.2	1.79	1.66	-7.3%	2.30	28.4%	149
Diethyl Ether	Acetone	388.3	1.66	1.50	-9.4%	2.82	70.3%	149
Diethyl Ether	Acetonitrile	298.1	3.38	3.74	10.7%	4.02	19.0%	148
Diethyl Ether	Acetonitrile	338.2	3.02	2.77	-8.3%	3.16	4.6%	148
Diethyl Ether	Acetonitrile	388.2	2.63	2.13	-19.1%	2.41	-8.4%	148
Diethyl Ether	Diethyl Phthalate	303.2	1.47	1.53	4.1%	1.13	-23.1%	[39]
Diethyl Ether	Diethyl Phthalate	313.2	1.46	1.49	2.1%	1.11	-24.0%	[39]
Diethyl Ether	Diethyl Phthalate	323.2	1.46	1.46	0.0%	1.10	-24.7%	[39]
Diethyl Ether	Diethyl Phthalate	333.2	1.46	1.43	-2.1%	1.10	-24.7%	[39]
Diethyl Ether	Epsilon-Caprolactone	303.2	3.09	3.52	13.9%	M.G.	N.A.	[41]
Diethyl Ether	Epsilon-Caprolactone	318.2	3.06	3.22	5.2%	M.G.	N.A.	[41]
Diethyl Ether	Epsilon-Caprolactone	333.2	3.01	2.98	-1.0%	M.G.	N.A.	[41]
Diethyl Ether	Ethyl Benzoate	313.2	1.29	1.38	7.0%	1.16	-10.1%	[41]
Diethyl Ether	Ethyl Benzoate	323.2	1.30	1.36	4.6%	1.15	-11.5%	[41]
Diethyl Ether	Ethyl Benzoate	333.2	1.30	1.35	3.8%	1.15	-11.5%	[41]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Diethyl Ether	Ethyl Benzoate	343.2	1.31	1.33	1.5%	1.15	-12.2%	[41]
Diethyl Ether	Glutaronitrile	303.2	6.32	6.94	9.8%	13.25	109.7%	[39]
Diethyl Ether	Glutaronitrile	313.2	6.24	6.26	0.3%	12.83	105.6%	[39]
Diethyl Ether	Glutaronitrile	323.2	6.18	5.69	-7.9%	12.41	100.8%	[39]
Diethyl Ether	Glutaronitrile	333.2	6.09	5.21	-14.4%	11.98	96.7%	[39]
Diethyl Ether	Methanol	298.2	3.47	3.24	-6.6%	4.27	23.1%	150
Diethyl Ether	Methanol	338.2	3.29	2.88	-12.6%	4.02	22.1%	150
Diethyl Ether	Methanol	388.2	2.98	2.34	-21.5%	3.62	21.4%	150
Diethyl Ether	N,N-Dibutylformamide	302.8	1.47	1.31	-10.6%	M.P.	N.A.	[13]
Diethyl Ether	N,N-Dibutylformamide	318.3	1.43	1.28	-10.6%	M.P.	N.A.	[13]
Diethyl Ether	N,N-Dibutylformamide	332.4	1.41	1.25	-11.5%	M.P.	N.A.	[13]
Diethyl Ether	N,N-Diethylacetamide	303.2	1.89	1.79	-5.3%	1.46	-22.8%	[39]
Diethyl Ether	N,N-Diethylacetamide	313.2	1.86	1.74	-6.5%	1.49	-19.9%	[39]
Diethyl Ether	N,N-Diethylacetamide	323.2	1.83	1.70	-7.1%	1.52	-16.9%	[39]
Diethyl Ether	N,N-Diethylacetamide	333.2	1.81	1.66	-8.3%	1.54	-14.9%	[39]
Diethyl Ether	N,N-Dimethylacetamide	303.4	3.24	2.86	-11.6%	3.11	-3.9%	[13]
Diethyl Ether	N,N-Dimethylacetamide	317.6	3.18	2.67	-16.0%	3.15	-0.8%	[13]
Diethyl Ether	N,N-Dimethylacetamide	333.6	3.13	2.49	-20.4%	3.19	1.9%	[13]
Diethyl Ether	N-Ethylacetamide	303.2	3.12	3.08	-1.3%	M.G.	N.A.	[39]
Diethyl Ether	N-Ethylacetamide	313.2	3.09	3.00	-2.9%	M.G.	N.A.	[39]
Diethyl Ether	N-Ethylacetamide	323.2	3.09	2.92	-5.5%	M.G.	N.A.	[39]
Diethyl Ether	N-Ethylacetamide	333.2	3.08	2.83	-8.1%	M.G.	N.A.	[39]
Diethyl Ether	N-Hexadecane	298.2	1.08	1.21	12.1%	1.02	-5.5%	[6]
Diethyl Ether	N-Methylacetamide	303.2	4.19	4.20	0.3%	M.P.	N.A.	[13]
Diethyl Ether	N-Methylacetamide	318.4	4.12	3.99	-3.2%	M.P.	N.A.	[13]
Diethyl Ether	N-Methylacetamide	333.2	4.06	3.77	-7.1%	M.P.	N.A.	[13]
Diethyl Ether	N-Methylformamide	303.2	6.55	6.54	-0.2%	M.P.	N.A.	[35]
Diethyl Ether	N-Methylformamide	313.2	6.44	6.17	-4.2%	M.P.	N.A.	[35]
Diethyl Ether	N-Methylformamide	323.2	6.34	5.81	-8.4%	M.P.	N.A.	[35]
Diethyl Ether	N-Methylformamide	333.2	6.25	5.47	-12.4%	M.P.	N.A.	[35]
Diethyl Ether	Sulfolane	303.8	6.59	7.80	18.4%	M.G.	N.A.	[13]
Diethyl Ether	Sulfolane	317.9	6.41	6.72	4.9%	M.G.	N.A.	[13]
Diethyl Ether	Sulfolane	333.6	6.21	5.81	-6.4%	M.G.	N.A.	[13]
Diethyl Ether	Tetraethylene Glycol DME	303.2	1.46	1.48	1.3%	1.08	-26.1%	[7]
Diethyl Ether	Tetraethylene Glycol DME	323.2	1.37	1.41	3.3%	1.06	-22.3%	[7]
Diethyl Ether	Tetraethylene Glycol DME	343.2	1.30	1.35	4.2%	1.04	-19.7%	[7]
Diethyl Ether	Toluene	293.2	1.12	1.23	9.8%	1.24	10.7%	[33]
Diethyl Ether	Toluene	293.2	1.10	1.23	11.8%	1.24	12.7%	[33]
Diethyl Ether	Toluene	293.2	1.01	1.23	21.8%	1.24	22.8%	[30]
Diethyl Ether	Toluene	303.2	1.12	1.23	9.8%	1.24	10.7%	[33]
Diethyl Ether	Toluene	303.2	1.01	1.23	21.8%	1.24	22.8%	[30]
Diethyl Ether	Toluene	313.2	1.24	1.22	-1.6%	1.24	0.0%	[33]
Diethyl Ether	Toluene	313.2	1.02	1.22	19.6%	1.24	21.6%	[30]
Diisopropyl Ether	1,5-Dimethyl-2-Pyrrolidinone	298.2	4.35	4.31	-0.9%	M.G.	N.A.	[29]
Diisopropyl Ether	1,5-Dimethyl-2-Pyrrolidinone	308.2	4.32	4.02	-6.9%	M.G.	N.A.	[29]
Diisopropyl Ether	1,5-Dimethyl-2-Pyrrolidinone	318.2	4.29	3.77	-12.1%	M.G.	N.A.	[29]
Diisopropyl Ether	1-Ethylpyrrolidin-2-One	298.2	4.70	4.35	-7.4%	M.P.	N.A.	[29]
Diisopropyl Ether	1-Ethylpyrrolidin-2-One	308.2	4.38	4.06	-7.3%	M.P.	N.A.	[29]
Diisopropyl Ether	1-Ethylpyrrolidin-2-One	318.2	4.19	3.80	-9.3%	M.P.	N.A.	[29]
Diisopropyl Ether	1-Octanol	298.2	1.79	1.42	-20.7%	1.91	6.7%	[3]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Diisopropyl Ether	2-Pyrrolidone	303.2	14.41	19.52	35.5%	M.G.	N.A.	[35]
Diisopropyl Ether	2-Pyrrolidone	313.2	13.91	16.88	21.4%	M.G.	N.A.	[35]
Diisopropyl Ether	2-Pyrrolidone	323.2	13.32	14.73	10.6%	M.G.	N.A.	[35]
Diisopropyl Ether	2-Pyrrolidone	333.2	12.92	12.96	0.3%	M.G.	N.A.	[35]
Diisopropyl Ether	Benzene	343.2	1.24	1.14	-8.0%	1.25	0.9%	60
Diisopropyl Ether	Benzyl Acetate	298.2	2.43	2.45	0.8%	2.24	-7.8%	[10]
Diisopropyl Ether	Carbon Tetrachloride	293.2	1.04	0.75	-27.9%	0.97	-6.7%	[10]
Diisopropyl Ether	Cyclohexane	313.2	1.27	1.45	14.2%	1.09	-14.2%	[56]
Diisopropyl Ether	Cyclohexane	333.2	1.23	1.41	14.6%	1.05	-14.6%	[56]
Diisopropyl Ether	Diethyl Phthalate	303.2	2.28	2.26	-0.9%	1.91	-16.2%	[39]
Diisopropyl Ether	Diethyl Phthalate	313.2	2.26	2.17	-4.0%	1.84	-18.6%	[39]
Diisopropyl Ether	Diethyl Phthalate	323.2	2.25	2.10	-6.7%	1.79	-20.4%	[39]
Diisopropyl Ether	Diethyl Phthalate	333.2	2.21	2.02	-8.6%	1.75	-20.8%	[39]
Diisopropyl Ether	Epsilon-Caprolactone	303.2	5.31	6.33	19.2%	M.G.	N.A.	[41]
Diisopropyl Ether	Epsilon-Caprolactone	318.2	5.21	5.51	5.8%	M.G.	N.A.	[41]
Diisopropyl Ether	Epsilon-Caprolactone	333.2	5.07	4.88	-3.7%	M.G.	N.A.	[41]
Diisopropyl Ether	Ethyl Benzoate	313.2	1.72	1.66	-3.5%	1.69	-1.7%	[41]
Diisopropyl Ether	Ethyl Benzoate	323.2	1.74	1.62	-6.9%	1.65	-5.2%	[41]
Diisopropyl Ether	Ethyl Benzoate	333.2	1.73	1.59	-8.1%	1.62	-6.4%	[41]
Diisopropyl Ether	Ethyl Benzoate	343.2	1.76	1.57	-10.8%	1.59	-9.7%	[41]
Diisopropyl Ether	Glutaronitrile	303.2	15.80	19.08	20.8%	42.59	169.6%	[39]
Diisopropyl Ether	Glutaronitrile	313.2	15.40	16.22	5.3%	39.09	153.8%	[39]
Diisopropyl Ether	Glutaronitrile	323.2	15.00	13.96	-6.9%	35.93	139.5%	[39]
Diisopropyl Ether	Glutaronitrile	333.2	14.60	12.17	-16.6%	33.08	126.6%	[39]
Diisopropyl Ether	N,N-Dibutylformamide	302.8	1.92	1.75	-8.7%	M.P.	N.A.	[13]
Diisopropyl Ether	N,N-Dibutylformamide	318.3	1.81	1.67	-7.6%	M.P.	N.A.	[13]
Diisopropyl Ether	N,N-Dibutylformamide	332.5	1.77	1.61	-9.1%	M.P.	N.A.	[13]
Diisopropyl Ether	N,N-Diethylacetamide	303.2	2.65	2.61	-1.5%	1.65	-37.7%	[39]
Diisopropyl Ether	N,N-Diethylacetamide	313.2	2.60	2.48	-4.6%	1.65	-36.5%	[39]
Diisopropyl Ether	N,N-Diethylacetamide	323.2	2.55	2.38	-6.7%	1.65	-35.3%	[39]
Diisopropyl Ether	N,N-Diethylacetamide	333.2	2.50	2.28	-8.8%	1.65	-34.0%	[39]
Diisopropyl Ether	N,N-Dimethylacetamide	303.2	4.04	4.78	18.2%	4.78	18.2%	[13]
Diisopropyl Ether	N,N-Dimethylacetamide	317.6	3.70	4.25	14.7%	4.55	22.8%	[13]
Diisopropyl Ether	N,N-Dimethylacetamide	333.0	3.40	3.81	12.0%	4.34	27.6%	[13]
Diisopropyl Ether	N-Ethylacetamide	303.2	4.79	4.39	-8.4%	M.G.	N.A.	[39]
Diisopropyl Ether	N-Ethylacetamide	323.2	4.75	4.06	-14.5%	M.G.	N.A.	[39]
Diisopropyl Ether	N-Ethylacetamide	333.2	4.72	3.89	-17.6%	M.G.	N.A.	[39]
Diisopropyl Ether	N-Heptane	313.2	1.18	1.22	3.4%	1.07	-9.3%	[56]
Diisopropyl Ether	N-Heptane	323.2	1.09	1.21	10.7%	1.06	-3.0%	283
Diisopropyl Ether	N-Heptane	333.2	1.17	1.19	1.7%	1.06	-9.4%	[56]
Diisopropyl Ether	N-Heptane	343.2	1.08	1.18	9.5%	1.05	-2.6%	283
Diisopropyl Ether	N-Hexadecane	298.2	1.17	1.15	-1.7%	0.97	-17.1%	[6]
Diisopropyl Ether	N-Methylacetamide	303.1	6.67	6.42	-3.7%	M.P.	N.A.	[13]
Diisopropyl Ether	N-Methylacetamide	318.4	6.48	5.95	-8.2%	M.P.	N.A.	[13]
Diisopropyl Ether	N-Methylacetamide	333.2	6.34	5.50	-13.2%	M.P.	N.A.	[13]
Diisopropyl Ether	N-Methylformamide	303.2	12.32	12.32	0.0%	M.P.	N.A.	[35]
Diisopropyl Ether	N-Methylformamide	313.2	12.08	11.28	-6.6%	M.P.	N.A.	[35]
Diisopropyl Ether	N-Methylformamide	323.2	11.89	10.32	-13.2%	M.P.	N.A.	[35]
Diisopropyl Ether	N-Methylformamide	333.2	11.70	9.44	-19.3%	M.P.	N.A.	[35]
Diisopropyl Ether	Quinoline	298.2	3.14	3.19	1.6%	M.G.	N.A.	[10]
Diisopropyl Ether	Sulfolane	303.8	14.45	19.48	34.8%	M.G.	N.A.	[13]
Diisopropyl Ether	Sulfolane	317.9	13.50	15.52	15.0%	M.G.	N.A.	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Diisopropyl Ether	Sulfolane	334.2	12.57	12.33	-1.9%	M.G.	N.A.	[13]
Diisopropyl Ether	Tetraethylene Glycol DME	303.2	2.17	2.32	6.9%	1.51	-30.4%	[7]
Diisopropyl Ether	Tetraethylene Glycol DME	323.2	2.10	2.14	2.1%	1.44	-31.3%	[7]
Diisopropyl Ether	Tetraethylene Glycol DME	343.2	2.06	1.99	-3.4%	1.38	-33.0%	[7]
Dimethyl Carbonate	1,1,1-Trichloroethane	298.2	1.64	1.81	10.3%	M.G.	N.A.	57
Dimethyl Carbonate	1,1,1-Trichloroethane	333.2	1.68	1.66	-1.3%	M.G.	N.A.	57
Dimethyl Carbonate	1-Propanol	313.2	5.09	5.40	6.1%	M.G.	N.A.	249
Dimethyl Carbonate	Benzene	283.2	1.60	1.47	-8.3%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	293.2	1.56	1.44	-7.5%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	313.2	1.48	1.40	-5.7%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	323.2	1.46	1.38	-5.7%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	333.2	1.44	1.36	-5.8%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	343.2	1.43	1.34	-6.1%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	363.2	1.40	1.31	-6.5%	M.G.	N.A.	239
Dimethyl Carbonate	Benzene	373.2	1.39	1.30	-6.5%	M.G.	N.A.	239
Dimethyl Carbonate	Cyclohexane	283.2	14.25	11.24	-21.1%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	293.2	11.23	9.70	-13.6%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	313.2	7.88	7.52	-4.5%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	323.2	6.84	6.73	-1.6%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	333.2	6.04	6.07	0.6%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	343.2	5.37	5.53	2.9%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	363.2	4.43	4.68	5.7%	M.G.	N.A.	240
Dimethyl Carbonate	Cyclohexane	373.2	4.05	4.35	7.4%	M.G.	N.A.	240
Dimethyl Carbonate	Ethanol	313.2	5.44	5.69	4.7%	M.G.	N.A.	250
Dimethyl Carbonate	Methanol	313.2	5.45	5.46	0.2%	M.G.	N.A.	251
Dimethyl Carbonate	Methyl Tert-Butyl Ether	298.2	2.22	3.35	50.7%	M.G.	N.A.	248
Dimethyl Carbonate	N-Heptane	283.2	10.51	12.91	22.9%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	293.2	8.81	11.06	25.5%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	313.2	6.56	8.45	28.8%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	323.2	5.78	7.52	30.2%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	333.2	5.14	6.75	31.3%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	343.2	4.61	6.11	32.4%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	363.2	3.79	5.12	35.0%	M.G.	N.A.	241
Dimethyl Carbonate	N-Heptane	373.2	3.47	4.73	36.4%	M.G.	N.A.	241
Dimethyl Carbonate	Toluene	318.2	1.71	1.63	-4.7%	M.G.	N.A.	306
Dimethyl Sulfoxide	Chloroform	293.2	0.07	0.12	61.1%	0.07	-6.0%	302
Dimethyl Sulfoxide	Chloroform	298.2	0.08	0.13	53.5%	0.08	-5.5%	302
Dimethyl Sulfoxide	Chloroform	308.2	0.11	0.16	49.8%	0.10	-6.4%	302
Dimethyl Sulfoxide	Chloroform	318.2	0.13	0.19	43.1%	0.13	-2.1%	302
Dimethyl Sulfoxide	Chloroform	328.2	0.16	0.22	36.3%	0.16	-0.9%	302
Dimethyl Sulfoxide	Dichloromethane	298.2	0.46	0.30	-34.8%	0.33	-28.3%	303
Dimethyl Sulfoxide	N-Hexadecane	298.2	116.10	112.82	-2.8%	41.98	-63.8%	[6]
Di-N-Propyl Ether	1-Butanol	278.2	2.96	2.83	-4.5%	2.81	-5.2%	72
Di-N-Propyl Ether	1-Butanol	288.2	2.87	2.79	-2.7%	2.75	-4.1%	72
Di-N-Propyl Ether	1-Butanol	293.2	2.85	2.76	-3.3%	2.72	-4.7%	72
Di-N-Propyl Ether	1-Butanol	298.2	2.77	2.73	-1.4%	2.69	-2.9%	72
Di-N-Propyl Ether	1-Butanol	303.2	2.74	2.70	-1.5%	2.66	-3.0%	72
Di-N-Propyl Ether	1-Butanol	308.2	2.68	2.67	-0.2%	2.64	-1.3%	72
Di-N-Propyl Ether	1-Butanol	313.2	2.65	2.64	-0.3%	2.62	-1.0%	72
Di-N-Propyl Ether	1-Butanol	323.2	2.58	2.57	-0.5%	2.57	-0.5%	72
Di-N-Propyl Ether	1-Octanol	293.2	1.92	2.31	20.2%	1.76	-8.4%	338
Di-N-Propyl Ether	1-Octanol	298.2	1.92	2.27	18.4%	1.74	-9.3%	338

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Di-N-Propyl Ether	1-Octanol	298.2	2.02	2.27	12.4%	1.74	-13.9%	[3]
Di-N-Propyl Ether	1-Octanol	303.2	1.90	2.23	17.7%	1.73	-8.7%	338
Di-N-Propyl Ether	1-Octanol	308.2	1.86	2.19	17.8%	1.71	-8.0%	338
Di-N-Propyl Ether	1-Octanol	313.2	1.85	2.15	16.3%	1.70	-8.0%	338
Di-N-Propyl Ether	1-Octanol	323.2	1.81	2.08	14.8%	1.67	-7.8%	338
Di-N-Propyl Ether	1-Propanol	278.2	3.53	3.28	-7.2%	3.46	-2.1%	451
Di-N-Propyl Ether	1-Propanol	288.2	3.48	3.22	-7.5%	3.38	-2.9%	451
Di-N-Propyl Ether	1-Propanol	293.2	3.50	3.19	-8.7%	3.35	-4.2%	451
Di-N-Propyl Ether	1-Propanol	298.2	3.37	3.15	-6.6%	3.31	-1.9%	451
Di-N-Propyl Ether	1-Propanol	303.2	3.35	3.11	-7.2%	3.28	-2.1%	451
Di-N-Propyl Ether	1-Propanol	308.2	3.36	3.07	-8.5%	3.25	-3.1%	451
Di-N-Propyl Ether	1-Propanol	313.2	3.31	3.03	-8.5%	3.21	-3.0%	451
Di-N-Propyl Ether	1-Propanol	323.2	3.19	2.94	-7.9%	3.15	-1.3%	451
Di-N-Propyl Ether	2-Butanol	288.2	3.03	2.69	-11.3%	2.75	-9.3%	71
Di-N-Propyl Ether	2-Butanol	293.2	2.90	2.66	-8.4%	2.72	-6.4%	71
Di-N-Propyl Ether	2-Butanol	298.2	2.84	2.63	-7.4%	2.69	-5.3%	71
Di-N-Propyl Ether	2-Butanol	303.2	2.76	2.59	-6.0%	2.66	-3.5%	71
Di-N-Propyl Ether	2-Butanol	308.2	2.73	2.56	-6.3%	2.64	-3.3%	71
Di-N-Propyl Ether	2-Methyl-1-Propanol	278.2	3.06	2.80	-8.6%	2.81	-8.3%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	288.2	2.92	2.75	-6.0%	2.75	-6.0%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	293.2	2.81	2.72	-3.2%	2.72	-3.2%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	298.2	2.80	2.69	-3.9%	2.69	-3.9%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	303.2	2.71	2.65	-2.4%	2.66	-2.0%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	308.2	2.64	2.62	-0.8%	2.64	-0.1%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	313.2	2.59	2.59	-0.2%	2.62	1.0%	70
Di-N-Propyl Ether	2-Methyl-1-Propanol	323.2	2.49	2.52	1.2%	2.57	3.2%	70
Di-N-Propyl Ether	2-Methyl-2-Propanol	298.2	2.73	2.26	-17.3%	1.79	-34.5%	69
Di-N-Propyl Ether	2-Methyl-2-Propanol	303.2	2.59	2.24	-13.4%	1.78	-31.2%	69
Di-N-Propyl Ether	2-Methyl-2-Propanol	308.2	2.53	2.21	-12.7%	1.76	-30.5%	69
Di-N-Propyl Ether	2-Methyl-2-Propanol	313.2	2.49	2.19	-11.9%	1.74	-30.0%	69
Di-N-Propyl Ether	2-Methyl-2-Propanol	318.2	2.42	2.16	-10.7%	1.73	-28.5%	69
Di-N-Propyl Ether	2-Methyl-2-Propanol	323.2	2.39	2.13	-11.0%	1.71	-28.6%	69
Di-N-Propyl Ether	Benzene	343.2	1.09	0.96	-12.2%	1.14	4.2%	304
Di-N-Propyl Ether	Carbon Tetrachloride	298.2	0.98	1.02	3.7%	0.90	-8.5%	139
Di-N-Propyl Ether	Chloroform	298.2	0.41	0.21	-48.3%	0.39	-3.9%	140
Di-N-Propyl Ether	Ethanol	308.2	4.57	3.93	-14.1%	4.50	-1.6%	337
Di-N-Propyl Ether	Ethanol	323.2	4.25	3.75	-11.7%	4.32	1.7%	337
Di-N-Propyl Ether	Ethanol	338.2	4.06	3.54	-12.8%	4.13	1.8%	337
Di-N-Propyl Ether	Ethylene Glycol Ethyl Ether	313.2	3.61	2.60	-27.9%	3.75	4.0%	348
Di-N-Propyl Ether	Ethylene Glycol Ethyl Ether	323.2	3.56	2.51	-29.5%	3.63	2.0%	348
Di-N-Propyl Ether	Ethylene Glycol Ethyl Ether	333.2	3.47	2.43	-30.0%	3.50	0.9%	348
Di-N-Propyl Ether	Isopropanol	278.2	3.96	3.28	-17.2%	2.79	-29.6%	451
Di-N-Propyl Ether	Isopropanol	288.2	3.73	3.22	-13.6%	2.73	-26.7%	451
Di-N-Propyl Ether	Isopropanol	293.2	3.68	3.19	-13.3%	2.70	-26.6%	451
Di-N-Propyl Ether	Isopropanol	298.2	3.57	3.16	-11.5%	2.67	-25.2%	451
Di-N-Propyl Ether	Isopropanol	303.2	3.52	3.12	-11.4%	2.65	-24.8%	451
Di-N-Propyl Ether	Isopropanol	308.2	3.46	3.08	-11.1%	2.62	-24.4%	451
Di-N-Propyl Ether	Isopropanol	313.2	3.36	3.04	-9.5%	2.59	-22.9%	451
Di-N-Propyl Ether	Isopropanol	323.2	3.27	2.95	-9.7%	2.54	-22.2%	451
Di-N-Propyl Ether	Methanol	278.2	7.85	5.58	-28.9%	7.20	-8.3%	74
Di-N-Propyl Ether	Methanol	288.2	7.05	5.55	-21.3%	7.03	-0.3%	74
Di-N-Propyl Ether	Methanol	293.2	7.02	5.50	-21.7%	6.94	-1.2%	74

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Di-N-Propyl Ether	Methanol	298.2	7.15	5.44	-23.9%	6.86	-4.0%	74
Di-N-Propyl Ether	Methanol	303.2	6.92	5.35	-22.7%	6.77	-2.2%	74
Di-N-Propyl Ether	Methanol	308.2	6.74	5.26	-22.0%	6.68	-1.0%	74
Di-N-Propyl Ether	Methanol	313.2	6.66	5.15	-22.7%	6.60	-0.9%	74
Di-N-Propyl Ether	Methanol	323.2	6.38	4.92	-22.9%	6.42	0.6%	74
Di-N-Propyl Ether	N-Heptane	343.2	1.10	2.04	86.2%	1.11	1.3%	305
Di-N-Propyl Ether	N-Hexadecane	298.2	1.21	2.19	81.4%	1.04	-13.8%	[6]
Dioxane	Diiodomethane	298.2	1.57	32.98	2000.6%	M.G.	N.A.	[16]
Ethanol	1,1-Dichloroethane	298.2	9.13	9.31	2.0%	11.69	28.0%	[16]
Ethanol	1,2-Dichloroethane	318.4	9.70	8.23	-15.2%	4.79	-50.6%	[12]
Ethanol	1,2-Dichloroethane	337.2	7.20	6.38	-11.4%	3.62	-49.7%	[12]
Ethanol	1,4-Dioxane	298.2	2.49	2.72	9.2%	2.54	2.0%	[16]
Ethanol	1,4-Dioxane	323.2	2.42	2.34	-3.2%	2.16	-10.7%	339
Ethanol	1,4-Dioxane	323.2	2.36	2.34	-0.7%	2.16	-8.3%	339
Ethanol	1-Butanol	298.2	0.93	1.06	14.0%	1.05	12.9%	[16]
Ethanol	1-Butanol	308.2	1.02	1.05	2.9%	1.05	2.9%	[30]
Ethanol	1-Butanol	313.2	1.06	1.05	-0.7%	1.05	-0.7%	4
Ethanol	1-Butanol	318.2	1.01	1.05	4.0%	1.05	4.0%	[30]
Ethanol	1-Butanol	328.2	1.00	1.04	4.0%	1.04	4.0%	[30]
Ethanol	1-Hexanol	333.2	1.58	1.10	-30.4%	1.10	-30.4%	[81]
Ethanol	1-Octanol	293.4	1.18	1.33	12.7%	1.19	0.8%	[31]
Ethanol	1-Octanol	298.2	1.26	1.31	4.0%	1.19	-5.6%	[3]
Ethanol	1-Octanol	298.2	1.14	1.31	14.9%	1.19	4.4%	[16]
Ethanol	1-Octanol	303.5	1.20	1.29	7.5%	1.18	-1.7%	[31]
Ethanol	1-Octanol	313.6	1.20	1.26	5.0%	1.18	-1.7%	[31]
Ethanol	1-Octanol	323.4	1.13	1.24	9.7%	1.17	3.5%	[31]
Ethanol	1-Pentanol	308.2	1.09	1.12	2.8%	1.08	-0.9%	[30]
Ethanol	1-Pentanol	313.2	1.12	1.12	0.0%	1.08	-3.6%	[33]
Ethanol	1-Pentanol	318.2	1.17	1.11	-5.1%	1.08	-7.7%	[30]
Ethanol	1-Pentanol	323.5	1.12	1.11	-0.9%	1.08	-3.6%	[33]
Ethanol	1-Pentanol	328.2	1.14	1.10	-3.5%	1.07	-6.1%	[30]
Ethanol	1-Phenyl-1-Butanone	298.1	4.21	4.59	9.0%	3.50	-16.9%	[34]
Ethanol	1-Propanol	298.2	0.92	1.03	12.0%	1.02	10.9%	[16]
Ethanol	1-Propanol	313.2	1.03	1.03	-0.2%	1.02	-1.2%	6
Ethanol	2,2,4-Trimethylpentane	293.2	46.00	56.66	23.2%	51.44	11.8%	[10]
Ethanol	2,2,4-Trimethylpentane	298.2	44.58	47.22	5.9%	44.79	0.5%	[16]
Ethanol	2,2,4-Trimethylpentane	301.8	45.10	41.68	-7.6%	40.66	-9.8%	[48]
Ethanol	2,2,4-Trimethylpentane	319.5	28.30	24.21	-14.5%	25.98	-8.2%	[48]
Ethanol	2,2,4-Trimethylpentane	319.7	28.00	24.08	-14.0%	25.86	-7.6%	[48]
Ethanol	2,2,4-Trimethylpentane	319.7	27.50	24.08	-12.4%	25.86	-6.0%	[48]
Ethanol	2,2,4-Trimethylpentane	332.2	20.80	17.43	-16.2%	19.33	-7.1%	[48]
Ethanol	2,2,4-Trimethylpentane	332.2	20.70	17.43	-15.8%	19.33	-6.6%	[48]
Ethanol	2,2,4-Trimethylpentane	333.2	18.11	17.01	-6.1%	18.90	4.4%	63
Ethanol	2,2,4-Trimethylpentane	350.7	12.80	11.60	-9.4%	12.95	1.2%	[48]
Ethanol	2,2,4-Trimethylpentane	351.0	13.20	11.53	-12.7%	12.87	-2.5%	[48]
Ethanol	2,6-Dimethylpyridine	298.2	0.72	1.08	50.0%	1.88	161.1%	[16]
Ethanol	2,6-Dimethylpyridine	313.2	0.91	1.06	16.8%	1.88	107.2%	169
Ethanol	2-Methyl-1-Propanol	313.2	1.04	1.06	1.8%	1.05	0.8%	16
Ethanol	2-Methyl-2-Propanol	313.2	0.79	1.04	30.8%	1.30	63.6%	10
Ethanol	2-Nitropropane	293.2	8.42	8.99	6.8%	7.37	-12.5%	[10]
Ethanol	2-Pyrrolidone	303.2	1.06	0.95	-10.4%	M.G.	N.A.	[35]
Ethanol	2-Pyrrolidone	313.2	1.05	0.94	-10.3%	M.G.	N.A.	[35]

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Ethanol	2-Pyrrolidone	323.2	1.04	0.93	-10.2%	M.G.	N.A.	[35]
Ethanol	2-Pyrrolidone	333.2	1.02	0.93	-9.2%	M.G.	N.A.	[35]
Ethanol	Acetic Acid	298.2	0.84	0.64	-23.8%	1.89	125.0%	[16]
Ethanol	Acetone	298.3	2.44	2.27	-7.0%	2.29	-6.1%	[17]
Ethanol	Acetone	303.3	2.32	2.21	-4.7%	2.21	-4.7%	[18]
Ethanol	Acetone	306.8	2.24	2.17	-3.1%	2.16	-3.6%	[12]
Ethanol	Acetone	308.2	2.24	2.16	-3.6%	2.14	-4.5%	[17]
Ethanol	Acetone	313.2	2.09	2.11	1.0%	2.07	-1.0%	[18]
Ethanol	Acetone	315.2	2.12	2.09	-1.4%	2.05	-3.3%	[12]
Ethanol	Acetone	318.4	2.07	2.06	-0.5%	2.01	-2.9%	[17]
Ethanol	Acetone	323.2	1.99	2.01	1.2%	1.95	-1.8%	215
Ethanol	Acetone	327.4	1.92	1.98	3.1%	1.91	-0.5%	[12]
Ethanol	Acetone	328.5	1.92	1.97	2.6%	1.89	-1.6%	[17]
Ethanol	Acetone	329.4	1.74	1.96	12.6%	1.88	8.0%	[11]
Ethanol	Acetonitrile	293.2	4.14	3.46	-16.4%	4.17	0.8%	206
Ethanol	Acetonitrile	298.2	3.90	3.34	-14.4%	3.95	1.3%	[16]
Ethanol	Acetonitrile	323.2	3.00	2.87	-4.4%	3.10	3.3%	206
Ethanol	Acetonitrile	343.2	2.54	2.59	1.8%	2.63	3.4%	206
Ethanol	Acetonitrile	393.2	1.81	2.12	16.9%	1.87	3.1%	206
Ethanol	Acetophenone	293.2	3.62	3.69	1.9%	3.55	-1.9%	[10]
Ethanol	Acetophenone	298.2	3.30	3.53	7.0%	3.40	3.0%	[16]
Ethanol	Aniline	298.2	2.40	2.62	9.2%	2.87	19.6%	[16]
Ethanol	Aniline	313.2	2.54	2.45	-3.5%	2.67	5.2%	36
Ethanol	Aniline	313.2	2.69	2.45	-8.9%	2.67	-0.7%	[66]
Ethanol	Aniline	328.2	2.45	2.30	-6.1%	2.47	0.8%	[66]
Ethanol	Aniline	350.8	2.17	2.11	-2.7%	2.19	1.0%	36
Ethanol	Aniline	386.7	1.88	1.88	0.2%	1.82	-3.0%	36
Ethanol	Anisole	293.2	10.00	11.16	11.6%	4.68	-53.2%	[10]
Ethanol	Anisole	298.2	8.45	10.15	20.1%	4.45	-47.3%	[16]
Ethanol	Benzene	298.2	16.90	19.21	13.7%	20.15	19.2%	[46]
Ethanol	Benzene	298.2	16.50	19.21	16.4%	20.15	22.1%	[46]
Ethanol	Benzene	298.2	15.18	19.21	26.5%	20.15	32.7%	[16]
Ethanol	Benzene	307.3	14.20	15.53	9.4%	15.73	10.8%	[48]
Ethanol	Benzene	307.3	14.40	15.53	7.8%	15.73	9.2%	[48]
Ethanol	Benzene	313.2	12.90	13.69	6.1%	13.56	5.1%	[46]
Ethanol	Benzene	317.4	11.90	12.57	5.6%	12.26	3.0%	[48]
Ethanol	Benzene	317.7	10.90	12.50	14.7%	12.18	11.7%	[48]
Ethanol	Benzene	321.0	10.10	11.72	16.0%	11.29	11.8%	[48]
Ethanol	Benzene	321.0	10.80	11.72	8.5%	11.29	4.5%	[48]
Ethanol	Benzene	337.3	7.80	8.81	12.9%	8.09	3.7%	[48]
Ethanol	Benzene	338.2	8.60	8.68	0.9%	7.96	-7.4%	[48]
Ethanol	Benzene	342.4	7.90	8.13	2.9%	7.38	-6.6%	[12]
Ethanol	Benzene	349.0	7.60	7.38	-2.9%	6.61	-13.0%	[12]
Ethanol	Benzene	352.2	5.80	7.05	21.6%	6.29	8.4%	[48]
Ethanol	Benzene	354.2	5.70	6.86	20.4%	6.10	7.0%	[48]
Ethanol	Benzonitrile	293.2	4.70	5.27	12.1%	M.G.	N.A.	[10]
Ethanol	Benzonitrile	298.2	4.59	4.94	7.6%	M.G.	N.A.	[16]
Ethanol	Benzyl Alcohol	298.2	1.02	1.05	2.9%	1.31	28.4%	[16]
Ethanol	Bromobenzene	298.2	17.18	18.12	5.5%	12.80	-25.5%	[16]
Ethanol	Butyl Ether	298.2	7.30	8.78	20.3%	6.11	-16.3%	[16]
Ethanol	Butyronitrile	278.2	4.32	4.40	1.8%	1.63	-62.3%	30
Ethanol	Butyronitrile	288.2	3.89	3.94	1.2%	1.63	-58.1%	30

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethanol	Butyronitrile	293.2	3.75	3.75	0.0%	1.62	-56.8%	30
Ethanol	Butyronitrile	298.2	3.55	3.57	0.5%	1.59	-55.3%	30
Ethanol	Butyronitrile	298.2	3.50	3.57	2.0%	1.59	-54.6%	[16]
Ethanol	Butyronitrile	303.2	3.36	3.42	1.7%	1.57	-53.3%	30
Ethanol	Butyronitrile	308.2	3.26	3.27	0.4%	1.54	-52.7%	30
Ethanol	Butyronitrile	313.2	3.12	3.14	0.8%	1.50	-51.9%	30
Ethanol	Butyronitrile	323.2	2.93	2.91	-0.6%	1.43	-51.1%	30
Ethanol	Carbon Disulfide	298.2	78.66	72.26	-8.1%	M.P.	N.A.	[16]
Ethanol	Carbon Disulfide	298.3	78.30	72.02	-8.0%	M.P.	N.A.	[17]
Ethanol	Carbon Disulfide	308.4	67.50	52.31	-22.5%	M.P.	N.A.	[17]
Ethanol	Carbon Disulfide	318.7	55.40	39.11	-29.4%	M.P.	N.A.	[17]
Ethanol	Carbon Tetrachloride	293.2	34.40	32.46	-5.6%	39.25	14.1%	[28]
Ethanol	Carbon Tetrachloride	298.2	27.84	27.99	0.5%	33.66	20.9%	[16]
Ethanol	Carbon Tetrachloride	313.2	19.40	18.84	-2.9%	22.04	13.6%	[28]
Ethanol	Carbon Tetrachloride	333.2	10.20	12.20	19.6%	13.52	32.5%	[28]
Ethanol	Chlorobenzene	298.2	15.59	20.80	33.4%	20.51	31.6%	[16]
Ethanol	Chloroform	298.2	5.24	6.76	29.0%	9.02	72.1%	[16]
Ethanol	Chloroform	316.0	4.49	5.25	16.9%	5.92	31.8%	[12]
Ethanol	Chloroform	323.2	6.29	4.80	-23.7%	5.09	-19.1%	201
Ethanol	Chloroform	323.2	6.19	4.80	-22.5%	5.09	-17.8%	201
Ethanol	Cyclohexane	293.2	66.60	70.43	5.8%	84.57	27.0%	[28]
Ethanol	Cyclohexane	298.2	63.70	58.73	-7.8%	71.56	12.3%	[16]
Ethanol	Cyclohexane	303.0	61.80	49.83	-19.4%	61.20	-1.0%	[48]
Ethanol	Cyclohexane	312.9	29.90	36.48	22.0%	44.85	50.0%	[17]
Ethanol	Cyclohexane	313.2	35.70	36.16	1.3%	44.44	24.5%	[28]
Ethanol	Cyclohexane	322.9	24.30	27.54	13.3%	33.28	37.0%	[17]
Ethanol	Cyclohexane	323.5	35.30	27.10	-23.2%	32.71	-7.3%	[48]
Ethanol	Cyclohexane	323.5	34.90	27.10	-22.3%	32.71	-6.3%	[48]
Ethanol	Cyclohexane	333.0	19.10	21.35	11.8%	25.00	30.9%	[17]
Ethanol	Cyclohexane	333.2	17.40	21.25	22.1%	24.87	42.9%	[28]
Ethanol	Cyclohexane	342.8	21.30	17.10	-19.7%	19.23	-9.7%	[48]
Ethanol	Cyclohexane	342.8	21.60	17.10	-20.8%	19.23	-11.0%	[48]
Ethanol	Cyclohexane	343.0	15.10	17.02	12.7%	19.13	26.7%	[17]
Ethanol	Cyclohexane	352.9	11.70	13.90	18.8%	14.90	27.4%	[17]
Ethanol	Cyclohexane	361.2	14.50	11.91	-17.9%	12.22	-15.7%	[48]
Ethanol	Cyclohexane	361.2	13.50	11.91	-11.8%	12.22	-9.5%	[48]
Ethanol	Cyclohexanone	298.2	2.06	2.19	6.3%	2.72	32.0%	[16]
Ethanol	Dichloromethane	298.2	9.21	8.24	-10.5%	10.56	14.7%	[16]
Ethanol	Diethyl Phthalate	303.2	2.80	2.84	1.4%	2.47	-11.8%	[39]
Ethanol	Diethyl Phthalate	313.2	2.58	2.60	0.8%	2.25	-12.8%	[39]
Ethanol	Diethyl Phthalate	323.2	2.40	2.39	-0.4%	2.07	-13.8%	[39]
Ethanol	Diethyl Phthalate	333.2	2.21	2.22	0.5%	1.91	-13.6%	[39]
Ethanol	Diiodomethane	298.2	32.45	4.11	-87.3%	M.G.	N.A.	[16]
Ethanol	Diisopropyl Ether	298.2	4.65	6.55	40.9%	7.79	67.5%	[16]
Ethanol	Dimethyl Carbonate	313.2	4.36	4.98	14.1%	M.G.	N.A.	250
Ethanol	Dimethyl Sulfoxide	298.2	0.53	0.45	-15.1%	0.59	11.3%	[16]
Ethanol	Di-N-Propyl Ether	308.2	6.50	6.56	0.9%	5.16	-20.6%	337
Ethanol	Di-N-Propyl Ether	323.2	5.69	5.22	-8.3%	4.60	-19.2%	337
Ethanol	Di-N-Propyl Ether	338.2	4.64	4.29	-7.4%	4.12	-11.1%	337
Ethanol	Epsilon-Caprolactone	303.2	2.00	1.92	-4.0%	M.G.	N.A.	[41]
Ethanol	Epsilon-Caprolactone	318.2	1.84	1.81	-1.6%	M.G.	N.A.	[41]
Ethanol	Epsilon-Caprolactone	333.2	1.66	1.73	4.2%	M.G.	N.A.	[41]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethanol	Ethyl Acetate	298.2	3.40	4.50	32.4%	2.90	-14.7%	[16]
Ethanol	Ethyl Acetate	313.0	2.84	3.81	34.2%	2.54	-10.6%	[12]
Ethanol	Ethyl Acetate	328.2	2.75	3.29	19.7%	2.27	-17.4%	235
Ethanol	Ethyl Acetate	328.4	2.55	3.29	29.0%	2.27	-11.0%	[17]
Ethanol	Ethyl Acetate	333.5	2.42	3.14	29.8%	2.19	-9.5%	[12]
Ethanol	Ethyl Acetate	338.4	2.44	3.02	23.8%	2.13	-12.7%	[17]
Ethanol	Ethyl Acetate	348.3	2.33	2.80	20.2%	2.01	-13.7%	[12]
Ethanol	Ethyl Acetate	349.1	2.34	2.78	18.8%	2.00	-14.5%	[17]
Ethanol	Ethylene Glycol Ethyl Ether	313.2	1.11	1.03	-7.1%	0.93	-16.1%	383
Ethanol	Glutaronitrile	303.2	4.12	3.71	-10.0%	5.98	45.1%	[39]
Ethanol	Glutaronitrile	313.2	3.72	3.44	-7.5%	5.45	46.5%	[39]
Ethanol	Glutaronitrile	323.2	3.40	3.21	-5.6%	4.99	46.8%	[39]
Ethanol	Glutaronitrile	333.2	3.12	3.01	-3.5%	4.60	47.4%	[39]
Ethanol	Isopropanol	298.2	0.88	1.03	17.0%	1.05	19.3%	[16]
Ethanol	M-Cresol	298.2	0.29	0.26	-10.3%	0.32	10.3%	[16]
Ethanol	Methanol	337.0	1.02	1.03	1.0%	0.97	-4.9%	[17]
Ethanol	Methyl Ethyl Ketone	278.2	3.01	3.15	4.8%	2.76	-8.2%	264
Ethanol	Methyl Ethyl Ketone	288.2	2.78	2.88	3.4%	2.55	-8.4%	264
Ethanol	Methyl Ethyl Ketone	298.2	2.59	2.66	2.6%	2.37	-8.6%	264
Ethanol	Methyl Ethyl Ketone	298.2	2.36	2.66	12.7%	2.37	0.4%	[16]
Ethanol	Methyl Ethyl Ketone	308.2	2.39	2.48	3.6%	2.22	-7.2%	264
Ethanol	Methyl Ethyl Ketone	313.0	2.24	2.41	7.6%	2.15	-4.0%	[18]
Ethanol	Methyl Ethyl Ketone	313.2	2.33	2.40	2.9%	2.15	-7.8%	264
Ethanol	Methyl Ethyl Ketone	313.2	2.18	2.40	10.1%	2.15	-1.4%	[18]
Ethanol	Methyl Ethyl Ketone	314.7	2.26	2.38	5.3%	2.13	-5.8%	[12]
Ethanol	Methyl Ethyl Ketone	323.2	2.17	2.26	4.3%	2.02	-6.8%	264
Ethanol	Methyl Ethyl Ketone	323.2	2.10	2.26	7.6%	2.02	-3.8%	[18]
Ethanol	Methyl Ethyl Ketone	333.1	1.98	2.14	8.1%	1.91	-3.5%	[18]
Ethanol	Methyl Ethyl Ketone	333.3	1.99	2.14	7.5%	1.91	-4.0%	[12]
Ethanol	Methyl Ethyl Ketone	348.6	1.74	1.99	14.4%	1.75	0.6%	[12]
Ethanol	Methyl Ethyl Ketone	352.8	1.75	1.95	11.4%	1.72	-1.7%	[11]
Ethanol	Methylcyclohexane	313.2	28.47	32.89	15.5%	39.52	38.8%	[56]
Ethanol	Methylcyclohexane	333.2	14.44	19.33	33.9%	22.76	57.6%	[56]
Ethanol	N,N-Dibutylformamide	302.8	0.83	0.84	1.3%	1.11	33.9%	[13]
Ethanol	N,N-Dibutylformamide	318.3	0.84	0.83	-0.8%	1.09	30.2%	[13]
Ethanol	N,N-Dibutylformamide	332.4	0.85	0.83	-1.8%	1.07	26.6%	[13]
Ethanol	N,N-Diethylacetamide	303.2	0.50	0.45	-10.2%	0.87	73.7%	[39]
Ethanol	N,N-Diethylacetamide	313.2	0.51	0.47	-7.8%	0.88	72.5%	[39]
Ethanol	N,N-Diethylacetamide	323.2	0.52	0.50	-3.5%	0.88	69.9%	[39]
Ethanol	N,N-Diethylacetamide	333.2	0.52	0.52	-0.8%	0.88	67.9%	[39]
Ethanol	N,N-Dimethylacetamide	303.6	0.53	0.49	-7.7%	0.61	14.9%	[13]
Ethanol	N,N-Dimethylacetamide	317.6	0.58	0.54	-6.9%	0.61	5.2%	[13]
Ethanol	N,N-Dimethylacetamide	333.6	0.63	0.59	-6.1%	0.62	-1.3%	[13]
Ethanol	N,N-Dimethylformamide	298.2	0.75	0.66	-12.0%	0.75	0.0%	[16]
Ethanol	N,N-Dimethylformamide	313.2	0.87	0.69	-21.0%	0.73	-16.4%	66
Ethanol	N-Decane	293.2	58.40	56.53	-3.2%	45.37	-22.3%	[23]
Ethanol	N-Decane	298.2	41.99	47.01	12.0%	39.51	-5.9%	[16]
Ethanol	N-Decane	306.4	37.50	35.54	-5.2%	31.78	-15.3%	[48]
Ethanol	N-Decane	321.4	25.50	22.68	-11.1%	21.90	-14.1%	[48]
Ethanol	N-Decane	333.2	15.50	16.72	7.9%	16.67	7.5%	[81]
Ethanol	N-Decane	338.7	15.90	14.69	-7.6%	14.76	-7.2%	[48]
Ethanol	N-Decane	343.2	15.60	13.28	-14.9%	13.39	-14.2%	[81]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethanol	N-Decane	357.5	10.90	9.93	-8.9%	9.94	-8.8%	[48]
Ethanol	N-Dodecane	293.2	55.90	55.30	-1.1%	40.95	-26.7%	[23]
Ethanol	N-Ethylacetamide	303.2	0.78	0.65	-16.3%	1.03	32.6%	[39]
Ethanol	N-Ethylacetamide	313.2	0.78	0.66	-15.2%	1.01	29.8%	[39]
Ethanol	N-Ethylacetamide	323.2	0.78	0.66	-15.6%	0.99	26.6%	[39]
Ethanol	N-Ethylacetamide	333.2	0.78	0.66	-15.8%	0.98	25.0%	[39]
Ethanol	N-Formylmorpholine	303.5	1.52	1.35	-11.2%	M.G.	N.A.	[43]
Ethanol	N-Formylmorpholine	323.2	1.41	1.29	-8.5%	M.G.	N.A.	[43]
Ethanol	N-Formylmorpholine	342.8	1.35	1.25	-7.4%	M.G.	N.A.	[43]
Ethanol	N-Heptane	288.2	83.40	71.65	-14.1%	64.19	-23.0%	[23]
Ethanol	N-Heptane	293.2	51.00	59.08	15.8%	55.65	9.1%	[10]
Ethanol	N-Heptane	293.2	67.90	59.08	-13.0%	55.65	-18.0%	[23]
Ethanol	N-Heptane	293.5	48.10	58.42	21.5%	55.18	14.7%	[28]
Ethanol	N-Heptane	298.2	49.22	49.27	0.1%	48.46	-1.5%	[16]
Ethanol	N-Heptane	298.2	58.80	49.27	-16.2%	48.46	-17.6%	[23]
Ethanol	N-Heptane	303.2	46.15	41.52	-10.0%	42.39	-8.1%	[23]
Ethanol	N-Heptane	303.2	49.70	41.52	-16.5%	42.39	-14.7%	[23]
Ethanol	N-Heptane	303.3	42.90	41.38	-3.5%	42.27	-1.5%	[28]
Ethanol	N-Heptane	303.3	34.20	41.35	20.9%	42.25	23.6%	141
Ethanol	N-Heptane	308.2	42.20	35.33	-16.3%	37.22	-11.8%	[23]
Ethanol	N-Heptane	313.1	31.80	30.42	-4.3%	32.88	3.4%	[28]
Ethanol	N-Heptane	313.2	27.74	30.33	9.3%	32.80	18.3%	141
Ethanol	N-Heptane	313.2	43.10	30.33	-29.6%	32.80	-23.9%	[18]
Ethanol	N-Heptane	313.2	39.94	30.33	-24.1%	32.80	-17.9%	[56]
Ethanol	N-Heptane	313.2	37.60	30.33	-19.3%	32.80	-12.8%	[23]
Ethanol	N-Heptane	314.5	36.30	29.19	-19.6%	31.76	-12.5%	[48]
Ethanol	N-Heptane	314.6	34.60	29.11	-15.9%	31.68	-8.4%	[48]
Ethanol	N-Heptane	318.2	32.00	26.26	-17.9%	29.01	-9.3%	[23]
Ethanol	N-Heptane	322.8	21.90	23.16	5.8%	25.98	18.6%	[28]
Ethanol	N-Heptane	323.2	24.72	22.92	-7.3%	25.74	4.1%	141
Ethanol	N-Heptane	323.2	32.60	22.92	-29.7%	25.74	-21.0%	[18]
Ethanol	N-Heptane	323.2	28.10	22.92	-18.4%	25.74	-8.4%	[23]
Ethanol	N-Heptane	332.2	23.20	18.26	-21.3%	20.91	-9.9%	[48]
Ethanol	N-Heptane	333.2	23.80	17.82	-25.1%	20.45	-14.1%	[18]
Ethanol	N-Heptane	333.2	16.27	17.82	9.5%	20.45	25.7%	[56]
Ethanol	N-Heptane	343.1	16.34	14.22	-13.0%	16.42	0.5%	141
Ethanol	N-Heptane	349.6	14.60	12.45	-14.7%	14.34	-1.8%	[48]
Ethanol	N-Heptane	349.6	15.10	12.45	-17.5%	14.34	-5.0%	[48]
Ethanol	N-Heptane	366.8	9.80	9.06	-7.6%	10.14	3.5%	[48]
Ethanol	N-Hexadecane	293.2	50.40	52.02	3.2%	34.76	-31.0%	[23]
Ethanol	N-Hexadecane	298.2	40.40	43.07	6.6%	30.27	-25.1%	[6]
Ethanol	N-Hexadecane	298.2	34.75	43.07	23.9%	30.27	-12.9%	[16]
Ethanol	N-Hexane	288.2	83.70	72.57	-13.3%	70.49	-15.8%	[23]
Ethanol	N-Hexane	293.2	69.90	59.90	-14.3%	61.12	-12.6%	[23]
Ethanol	N-Hexane	297.2	62.60	51.79	-17.3%	54.70	-12.6%	[48]
Ethanol	N-Hexane	297.4	58.20	51.43	-11.6%	54.40	-6.5%	[48]
Ethanol	N-Hexane	297.7	59.40	50.88	-14.3%	53.96	-9.2%	[48]
Ethanol	N-Hexane	298.2	55.35	50.00	-9.7%	53.22	-3.8%	[16]
Ethanol	N-Hexane	298.2	60.10	50.00	-16.8%	53.22	-11.4%	[23]
Ethanol	N-Hexane	303.2	51.50	42.17	-18.1%	46.55	-9.6%	[23]
Ethanol	N-Hexane	304.8	38.00	40.02	5.3%	44.63	17.4%	[12]
Ethanol	N-Hexane	308.2	43.80	35.92	-18.0%	40.87	-6.7%	[23]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethanol	N-Hexane	313.2	32.50	30.87	-5.0%	36.02	10.8%	[18]
Ethanol	N-Hexane	313.2	38.30	30.87	-19.4%	36.02	-6.0%	[23]
Ethanol	N-Hexane	316.6	37.60	27.98	-25.6%	33.12	-11.9%	[48]
Ethanol	N-Hexane	316.7	35.40	27.90	-21.2%	33.04	-6.7%	[48]
Ethanol	N-Hexane	318.2	33.90	26.75	-21.1%	31.86	-6.0%	[23]
Ethanol	N-Hexane	322.6	33.00	23.73	-28.1%	28.67	-13.1%	[12]
Ethanol	N-Hexane	333.3	23.00	18.15	-21.1%	22.40	-2.6%	[18]
Ethanol	N-Hexane	334.0	21.90	17.86	-18.4%	22.06	0.7%	[48]
Ethanol	N-Hexane	334.0	22.40	17.86	-20.3%	22.06	-1.5%	[48]
Ethanol	N-Hexane	351.5	14.70	12.27	-16.5%	15.14	3.0%	[48]
Ethanol	N-Hexane	351.6	14.80	12.25	-17.2%	15.11	2.1%	[48]
Ethanol	Nitrobenzene	293.2	10.70	11.11	3.8%	11.38	6.4%	[10]
Ethanol	Nitrobenzene	298.2	9.16	10.14	10.7%	10.81	18.0%	[16]
Ethanol	Nitroethane	293.2	6.73	7.06	4.9%	7.51	11.6%	[10]
Ethanol	Nitromethane	298.2	8.24	6.79	-17.6%	8.47	2.8%	[16]
Ethanol	Nitromethane	298.2	9.37	6.79	-27.5%	8.47	-9.6%	196
Ethanol	Nitromethane	348.2	4.35	4.13	-5.0%	4.39	1.0%	196
Ethanol	Nitromethane	398.2	2.61	2.98	14.3%	2.94	12.8%	196
Ethanol	N-Methyl-2-Pyrrolidone	323.4	0.66	0.41	-38.0%	0.50	-24.4%	[43]
Ethanol	N-Methyl-2-Pyrrolidone	333.2	0.64	0.44	-31.1%	0.45	-29.6%	[43]
Ethanol	N-Methyl-2-Pyrrolidone	343.4	0.64	0.48	-25.3%	0.40	-37.8%	[43]
Ethanol	N-Methylacetamide	303.4	0.90	0.76	-15.9%	0.93	2.9%	[13]
Ethanol	N-Methylacetamide	313.2	0.87	0.76	-12.5%	0.92	5.9%	253
Ethanol	N-Methylacetamide	318.4	0.87	0.76	-12.8%	0.91	4.4%	[13]
Ethanol	N-Methylacetamide	332.8	0.85	0.76	-10.7%	0.91	6.9%	[13]
Ethanol	N-Methylformamide	303.2	1.31	1.21	-7.5%	M.P.	N.A.	254
Ethanol	N-Methylformamide	303.2	1.38	1.21	-12.3%	M.P.	N.A.	[35]
Ethanol	N-Methylformamide	313.2	1.34	1.20	-10.5%	M.P.	N.A.	254
Ethanol	N-Methylformamide	313.2	1.32	1.20	-9.0%	M.P.	N.A.	[35]
Ethanol	N-Methylformamide	323.2	1.27	1.19	-5.9%	M.P.	N.A.	[35]
Ethanol	N-Methylformamide	333.2	1.22	1.18	-3.5%	M.P.	N.A.	[35]
Ethanol	N-Nonane	296.1	50.70	51.60	1.8%	44.41	-12.4%	[48]
Ethanol	N-Nonane	296.1	51.70	51.60	-0.2%	44.41	-14.1%	[48]
Ethanol	N-Nonane	302.4	42.40	41.34	-2.5%	37.46	-11.7%	[48]
Ethanol	N-Nonane	312.3	32.60	30.10	-7.7%	29.02	-11.0%	[48]
Ethanol	N-Nonane	312.4	32.30	30.01	-7.1%	28.95	-10.4%	[48]
Ethanol	N-Nonane	315.0	30.40	27.77	-8.7%	27.14	-10.7%	[48]
Ethanol	N-Nonane	315.5	30.40	27.36	-10.0%	26.81	-11.8%	[48]
Ethanol	N-Nonane	323.7	23.80	21.76	-8.6%	22.01	-7.5%	[48]
Ethanol	N-Nonane	323.7	24.20	21.76	-10.1%	22.01	-9.0%	[48]
Ethanol	N-Nonane	333.2	16.50	17.10	3.6%	17.69	7.2%	[81]
Ethanol	N-Nonane	333.9	18.60	16.82	-9.6%	17.41	-6.4%	[48]
Ethanol	N-Nonane	334.0	18.80	16.78	-10.7%	17.38	-7.6%	[48]
Ethanol	N-Nonane	355.5	11.50	10.58	-8.0%	10.99	-4.4%	[48]
Ethanol	N-Nonane	355.5	11.40	10.58	-7.2%	10.99	-3.6%	[48]
Ethanol	N-Octane	288.2	77.80	70.64	-9.2%	59.39	-23.7%	[23]
Ethanol	N-Octane	293.2	50.50	58.19	15.2%	51.49	2.0%	[10]
Ethanol	N-Octane	293.2	64.10	58.19	-9.2%	51.49	-19.7%	[23]
Ethanol	N-Octane	298.2	55.40	48.48	-12.5%	44.84	-19.1%	[23]
Ethanol	N-Octane	303.2	47.60	40.81	-14.3%	39.21	-17.6%	[23]
Ethanol	N-Octane	308.2	41.10	34.70	-15.6%	34.43	-16.2%	[23]
Ethanol	N-Octane	313.2	36.20	29.77	-17.8%	30.35	-16.2%	[36]

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Ethanol	N-Octane	313.2	35.90	29.77	-17.1%	30.35	-15.5%	[23]
Ethanol	N-Octane	318.2	31.10	25.75	-17.2%	26.84	-13.7%	[23]
Ethanol	N-Octane	323.2	27.40	22.45	-18.1%	23.81	-13.1%	[23]
Ethanol	N-Octane	333.2	18.60	17.43	-6.3%	18.92	1.7%	[81]
Ethanol	N-Octane	333.2	27.70	17.43	-37.1%	18.92	-31.7%	[36]
Ethanol	N-Octane	343.2	17.48	13.89	-20.5%	15.19	-13.1%	336
Ethanol	N-Pentane	309.7	47.00	34.95	-25.6%	44.34	-5.7%	[48]
Ethanol	N-Pentane	310.2	49.50	34.43	-30.4%	43.79	-11.5%	[48]
Ethanol	N-Pentane	323.7	33.00	23.55	-28.6%	31.49	-4.6%	[48]
Ethanol	N-Pentane	338.7	21.00	16.42	-21.8%	22.41	6.7%	[48]
Ethanol	N-Pentane	339.2	23.00	16.24	-29.4%	22.16	-3.7%	[48]
Ethanol	N-Tetradecane	293.2	53.40	53.56	0.3%	37.52	-29.7%	[23]
Ethanol	P-Xylene	298.2	15.60	23.23	48.9%	16.87	8.1%	[16]
Ethanol	P-Xylene	313.2	15.48	15.81	2.2%	11.93	-22.9%	96
Ethanol	Pyridine	298.2	0.80	1.03	28.8%	0.78	-2.5%	[16]
Ethanol	Pyridine	313.2	1.13	1.03	-9.2%	0.81	-28.6%	185
Ethanol	Sulfolane	303.8	3.30	2.73	-17.4%	M.G.	N.A.	[13]
Ethanol	Sulfolane	317.9	2.89	2.53	-12.5%	M.G.	N.A.	[13]
Ethanol	Sulfolane	332.8	2.34	2.35	0.5%	M.G.	N.A.	[13]
Ethanol	Tetraethylene Glycol DME	303.2	1.19	1.05	-11.5%	1.12	-5.6%	[7]
Ethanol	Tetraethylene Glycol DME	323.2	1.14	1.00	-12.0%	1.01	-11.2%	[7]
Ethanol	Tetraethylene Glycol DME	343.2	1.02	0.96	-5.8%	0.94	-7.8%	[7]
Ethanol	Toluene	293.2	17.34	22.81	31.5%	20.66	19.1%	[33]
Ethanol	Toluene	293.2	17.98	22.81	26.9%	20.66	14.9%	[33]
Ethanol	Toluene	293.2	18.90	22.81	20.7%	20.66	9.3%	[30]
Ethanol	Toluene	293.2	18.40	22.81	24.0%	20.66	12.3%	[10]
Ethanol	Toluene	293.2	20.40	22.81	11.8%	20.66	1.3%	[24]
Ethanol	Toluene	298.2	15.43	19.99	29.6%	18.04	16.9%	[16]
Ethanol	Toluene	301.5	14.90	18.39	23.4%	16.56	11.1%	[48]
Ethanol	Toluene	301.8	15.00	18.26	21.7%	16.43	9.5%	[48]
Ethanol	Toluene	303.2	16.91	17.64	4.3%	15.86	-6.2%	211
Ethanol	Toluene	303.2	15.17	17.64	16.3%	15.86	4.5%	[33]
Ethanol	Toluene	303.2	14.70	17.64	20.0%	15.86	7.9%	[30]
Ethanol	Toluene	303.2	16.40	17.64	7.6%	15.86	-3.3%	[24]
Ethanol	Toluene	313.2	14.08	14.03	-0.4%	12.52	-11.1%	211
Ethanol	Toluene	313.2	14.90	14.03	-5.8%	12.52	-16.0%	[33]
Ethanol	Toluene	313.2	10.80	14.03	29.9%	12.52	15.9%	[30]
Ethanol	Toluene	313.2	13.50	14.03	3.9%	12.52	-7.3%	[24]
Ethanol	Toluene	323.2	11.80	11.43	-3.2%	10.13	-14.2%	211
Ethanol	Toluene	323.2	11.50	11.43	-0.6%	10.13	-11.9%	[24]
Ethanol	Toluene	333.2	9.93	9.50	-4.4%	8.39	-15.5%	211
Ethanol	Toluene	334.0	9.10	9.37	3.0%	8.27	-9.1%	[48]
Ethanol	Toluene	334.2	9.20	9.34	1.5%	8.24	-10.4%	[48]
Ethanol	Toluene	342.7	6.95	8.11	16.7%	7.15	2.9%	[12]
Ethanol	Toluene	353.7	6.10	6.88	12.8%	6.08	-0.3%	[48]
Ethanol	Toluene	354.2	6.30	6.83	8.4%	6.04	-4.1%	[48]
Ethanol	Toluene	381.0	4.39	4.89	11.4%	4.46	1.6%	[12]
Ethanol	Tributyl Phosphate	298.6	0.52	0.64	23.1%	M.G.	N.A.	[27]
Ethanol	Tributyl Phosphate	302.9	0.52	0.64	23.1%	M.G.	N.A.	[27]
Ethanol	Tributyl Phosphate	308.6	0.52	0.63	21.2%	M.G.	N.A.	[27]
Ethanol	Tributyl Phosphate	313.1	0.53	0.63	18.9%	M.G.	N.A.	[27]
Ethanol	Tributyl Phosphate	323.7	0.49	0.62	26.5%	M.G.	N.A.	[27]

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Ethanol	Tributyl Phosphate	330.0	0.48	0.62	29.2%	M.G.	N.A.	[27]
Ethanol	Triethylamine	298.2	1.96	4.79	144.4%	4.61	135.2%	[16]
Ethyl Acetate	1,2-Dichloroethane	318.4	0.83	0.82	-1.2%	0.52	-37.3%	[12]
Ethyl Acetate	1-Butanol	308.2	2.43	2.33	-4.1%	2.16	-11.1%	[30]
Ethyl Acetate	1-Butanol	318.2	2.30	2.26	-1.7%	2.01	-12.6%	[30]
Ethyl Acetate	1-Butanol	328.2	2.09	2.20	5.3%	1.89	-9.6%	[30]
Ethyl Acetate	1-Chlorobutane	323.2	1.25	1.21	-3.0%	1.18	-5.4%	[25]
Ethyl Acetate	1-Chlorobutane	348.2	1.23	1.18	-4.0%	1.16	-5.6%	[25]
Ethyl Acetate	1-Octanol	293.2	2.37	2.27	-4.2%	2.12	-10.5%	[10]
Ethyl Acetate	1-Octanol	298.2	2.48	2.21	-10.9%	2.01	-19.0%	[3]
Ethyl Acetate	1-Pentanol	303.5	2.49	2.32	-6.8%	2.14	-14.1%	[33]
Ethyl Acetate	1-Pentanol	313.2	2.32	2.24	-3.4%	1.98	-14.7%	[33]
Ethyl Acetate	1-Pentanol	323.5	2.15	2.17	0.9%	1.83	-14.9%	[33]
Ethyl Acetate	1-Phenyl-1-Butanone	298.1	1.35	1.10	-18.5%	1.14	-15.6%	[34]
Ethyl Acetate	2,2,4-Trimethylpentane	293.2	3.12	3.49	11.9%	3.50	12.2%	[10]
Ethyl Acetate	Acetic Acid	313.2	1.17	1.10	-6.0%	1.25	6.8%	[57]
Ethyl Acetate	Acetic Acid	333.2	1.21	1.08	-10.7%	1.27	5.0%	[57]
Ethyl Acetate	Acetic Acid	353.2	1.25	1.07	-14.4%	1.29	3.2%	[57]
Ethyl Acetate	Acetic Acid	373.2	1.29	1.05	-18.6%	1.30	0.8%	[57]
Ethyl Acetate	Acetonitrile	293.2	1.58	1.72	8.9%	1.78	12.7%	[10]
Ethyl Acetate	Acetonitrile	313.2	1.53	1.60	4.3%	1.77	15.4%	333
Ethyl Acetate	Acetonitrile	353.2	1.51	1.41	-6.4%	1.70	12.9%	333
Ethyl Acetate	Acetonitrile	393.2	1.48	1.29	-12.7%	1.62	9.6%	333
Ethyl Acetate	Aniline	293.2	1.44	1.38	-4.2%	0.71	-50.7%	[10]
Ethyl Acetate	Anisole	293.2	1.08	1.08	0.0%	0.86	-20.4%	[10]
Ethyl Acetate	Benzene	328.2	1.43	1.17	-18.2%	1.14	-20.3%	229
Ethyl Acetate	Benzyl Acetate	298.2	1.00	1.06	6.0%	1.16	16.0%	[10]
Ethyl Acetate	Butanal	298.2	1.13	1.01	-10.6%	1.03	-9.2%	[38]
Ethyl Acetate	Butanal	323.2	1.12	1.01	-9.8%	0.99	-11.3%	[38]
Ethyl Acetate	Butanal	347.2	1.09	1.01	-7.3%	0.97	-11.1%	[38]
Ethyl Acetate	Chlorobenzene	313.2	1.07	1.28	19.3%	1.04	-3.1%	39
Ethyl Acetate	Chlorobenzene	353.2	1.12	1.24	11.2%	1.11	-0.5%	39
Ethyl Acetate	Chlorobenzene	393.2	1.14	1.21	6.0%	1.07	-6.3%	39
Ethyl Acetate	Chloroform	313.2	0.16	0.31	95.7%	0.29	83.1%	231
Ethyl Acetate	Chloroform	323.2	0.21	0.34	59.4%	0.32	50.1%	231
Ethyl Acetate	Cyclohexane	313.2	3.33	3.93	18.0%	3.41	2.4%	[19]
Ethyl Acetate	Cyclohexane	328.2	3.18	3.54	11.3%	3.02	-5.0%	230
Ethyl Acetate	Cyclohexane	333.2	2.95	3.43	16.3%	2.91	-1.4%	[19]
Ethyl Acetate	Cyclohexanone	293.2	1.26	1.08	-14.3%	1.21	-4.0%	[10]
Ethyl Acetate	Dichloromethane	298.2	0.73	0.48	-34.7%	0.44	-40.1%	222
Ethyl Acetate	Dichloromethane	348.2	0.70	0.60	-14.3%	0.52	-25.8%	222
Ethyl Acetate	Dichloromethane	398.2	0.67	0.68	2.0%	0.56	-16.0%	222
Ethyl Acetate	Ethanol	298.2	3.61	2.86	-20.8%	2.76	-23.5%	[30]
Ethyl Acetate	Ethanol	328.2	2.62	2.65	1.0%	2.31	-11.9%	235
Ethyl Acetate	Ethylene Glycol Ethyl Ether	313.2	1.84	1.63	-11.5%	1.40	-24.0%	391
Ethyl Acetate	Isopropanol	288.2	3.55	2.63	-25.9%	2.37	-33.2%	[79]
Ethyl Acetate	Isopropanol	328.2	1.96	2.35	19.9%	1.78	-9.2%	236
Ethyl Acetate	Methyl Ethyl Ketone	314.7	1.11	1.02	-8.1%	1.11	0.0%	[12]
Ethyl Acetate	Methyl Ethyl Ketone	333.3	1.10	1.02	-7.3%	1.11	0.9%	[12]
Ethyl Acetate	Methyl Ethyl Ketone	348.6	1.10	1.01	-8.2%	1.11	0.9%	[10]
Ethyl Acetate	Methyl Isobutyl Ketone	328.2	1.22	1.03	-15.6%	1.11	-9.0%	[49]
Ethyl Acetate	Methyl Isobutyl Ketone	348.2	1.16	1.02	-12.1%	1.10	-5.2%	[49]

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Ethyl Acetate	Methyl Isobutyl Ketone	388.2	1.09	1.02	-6.4%	1.10	0.9%	[49]
Ethyl Acetate	N,N-Dibutylformamide	302.8	1.36	1.03	-24.0%	1.62	19.6%	[13]
Ethyl Acetate	N,N-Dibutylformamide	318.3	1.28	1.02	-20.4%	1.57	22.5%	[13]
Ethyl Acetate	N,N-Dibutylformamide	332.4	1.24	1.01	-18.2%	1.54	24.7%	[13]
Ethyl Acetate	N,N-Dimethylacetamide	303.3	1.81	1.40	-22.7%	1.82	0.6%	[13]
Ethyl Acetate	N,N-Dimethylacetamide	317.6	1.65	1.37	-16.9%	1.77	7.4%	[13]
Ethyl Acetate	N,N-Dimethylacetamide	333.6	1.50	1.34	-10.5%	1.65	10.1%	[13]
Ethyl Acetate	N,N-Dimethylformamide	313.2	1.62	1.79	10.4%	1.83	12.9%	80
Ethyl Acetate	N,N-Dimethylformamide	333.2	1.63	1.69	3.6%	1.80	10.3%	80
Ethyl Acetate	N-Formylmorpholine	303.5	2.48	2.51	1.2%	M.G.	N.A.	[43]
Ethyl Acetate	N-Formylmorpholine	323.2	2.36	2.31	-2.1%	M.G.	N.A.	[43]
Ethyl Acetate	N-Formylmorpholine	342.8	2.18	2.15	-1.4%	M.G.	N.A.	[43]
Ethyl Acetate	N-Heptane	293.2	3.29	3.66	11.2%	3.58	8.8%	[10]
Ethyl Acetate	N-Heptane	323.2	2.83	2.94	3.9%	2.83	0.0%	153
Ethyl Acetate	N-Heptane	343.2	2.53	2.62	3.4%	2.47	-2.5%	153
Ethyl Acetate	N-Hexadecane	298.2	2.90	2.90	0.0%	2.76	-4.8%	[6]
Ethyl Acetate	N-Hexane	298.1	3.39	3.56	5.0%	3.51	3.5%	[12]
Ethyl Acetate	N-Hexane	316.0	2.95	3.13	6.1%	3.05	3.4%	[12]
Ethyl Acetate	N-Hexane	332.0	2.60	2.83	8.8%	2.72	4.6%	[12]
Ethyl Acetate	N-Hexane	339.4	2.39	2.72	13.8%	2.59	8.4%	[12]
Ethyl Acetate	Nitrobenzene	293.2	1.38	1.12	-18.8%	M.P.	N.A.	[10]
Ethyl Acetate	Nitromethane	298.2	1.65	1.56	-5.7%	1.51	-8.7%	193
Ethyl Acetate	Nitromethane	348.2	1.53	1.37	-10.7%	1.45	-5.5%	193
Ethyl Acetate	Nitromethane	398.2	1.46	1.25	-14.6%	1.41	-3.7%	193
Ethyl Acetate	N-Methylacetamide	304.2	2.79	2.81	0.6%	2.91	4.2%	[13]
Ethyl Acetate	N-Methylacetamide	318.4	2.76	2.73	-1.2%	2.87	3.8%	[13]
Ethyl Acetate	N-Methylacetamide	331.9	2.72	2.64	-3.0%	2.82	3.6%	[13]
Ethyl Acetate	N-Octane	293.2	3.25	3.59	10.5%	3.50	7.7%	[10]
Ethyl Acetate	N-Octane	313.2	2.94	3.09	5.1%	2.98	1.4%	[36]
Ethyl Acetate	N-Octane	333.2	2.81	2.72	-3.2%	2.58	-8.2%	[36]
Ethyl Acetate	Propionitrile	293.2	1.44	1.32	-8.3%	1.26	-12.5%	[10]
Ethyl Acetate	P-Xylene	293.2	1.33	1.37	3.0%	1.59	19.5%	[10]
Ethyl Acetate	Quinoline	298.2	1.49	1.52	2.0%	M.G.	N.A.	[10]
Ethyl Acetate	Sulfolane	303.1	2.78	2.77	-0.4%	M.G.	N.A.	[13]
Ethyl Acetate	Sulfolane	317.9	2.67	2.56	-4.1%	M.G.	N.A.	[13]
Ethyl Acetate	Sulfolane	332.6	2.51	2.39	-4.9%	M.G.	N.A.	[13]
Ethyl Acetate	Tetraethylene Glycol DME	303.2	0.89	0.92	3.6%	0.72	-18.9%	[7]
Ethyl Acetate	Tetraethylene Glycol DME	323.2	0.86	0.91	5.3%	0.75	-13.2%	[7]
Ethyl Acetate	Tetraethylene Glycol DME	343.2	0.86	0.91	6.1%	0.78	-9.1%	[7]
Ethyl Acetate	Tetrahydrofuran	313.2	1.10	1.11	0.9%	1.11	0.9%	[19]
Ethyl Acetate	Tetrahydrofuran	333.2	1.10	1.10	0.0%	1.11	0.9%	[19]
Ethyl Acetate	Toluene	293.2	1.28	1.30	1.6%	1.36	6.3%	[10]
Ethyl Acetate	Toluene	342.7	1.16	1.25	7.8%	1.32	13.8%	[12]
Ethyl Acetate	Toluene	362.7	1.21	1.24	2.5%	1.29	6.6%	[12]
Ethyl Acetate	Toluene	380.9	1.20	1.22	1.7%	1.26	5.0%	[12]
Ethyl Acetate	Tributyl Phosphate	298.6	0.93	0.67	-28.0%	M.G.	N.A.	[27]
Ethyl Acetate	Tributyl Phosphate	302.9	0.93	0.67	-28.0%	M.G.	N.A.	[27]
Ethyl Acetate	Tributyl Phosphate	308.6	0.93	0.67	-28.0%	M.G.	N.A.	[27]
Ethyl Acetate	Tributyl Phosphate	313.1	0.95	0.67	-29.5%	M.G.	N.A.	[27]
Ethyl Iodide	1,2-Dichloroethane	293.2	1.38	1.21	-12.3%	0.95	-31.2%	[10]
Ethyl Iodide	1-Butanol	293.2	3.44	3.34	-2.9%	3.60	4.7%	[10]
Ethyl Iodide	1-Chlorobutane	293.2	1.29	1.16	-10.1%	M.P.	N.A.	[10]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethyl Iodide	1-Octanol	293.2	2.29	2.16	-5.7%	2.25	-1.7%	[10]
Ethyl Iodide	2,2,4-Trimethylpentane	293.2	1.87	2.30	23.0%	1.86	-0.5%	[10]
Ethyl Iodide	2-Nitropropane	293.2	2.22	2.14	-3.6%	2.21	-0.5%	[10]
Ethyl Iodide	Acetone	307.9	2.18	2.22	1.8%	1.82	-16.5%	[12]
Ethyl Iodide	Acetone	315.4	2.13	2.17	1.9%	1.79	-16.0%	[12]
Ethyl Iodide	Acetone	336.4	2.04	2.06	1.0%	1.71	-16.2%	[12]
Ethyl Iodide	Acetonitrile	293.2	5.14	5.66	10.1%	M.P.	N.A.	[10]
Ethyl Iodide	Acetophenone	293.2	1.42	1.47	3.5%	1.50	5.6%	[10]
Ethyl Iodide	Aniline	293.2	2.83	2.75	-2.8%	M.P.	N.A.	[10]
Ethyl Iodide	Anisole	293.2	1.12	1.15	2.7%	0.98	-12.5%	[10]
Ethyl Iodide	Benzene	293.2	1.13	1.02	-9.7%	1.08	-4.4%	[58]
Ethyl Iodide	Benzene	293.2	1.12	1.02	-8.9%	1.08	-3.6%	[10]
Ethyl Iodide	Benzyl Acetate	298.2	1.32	1.25	-5.3%	1.12	-15.2%	[10]
Ethyl Iodide	Carbon Tetrachloride	293.2	1.35	1.12	-17.0%	1.26	-6.7%	[10]
Ethyl Iodide	Cyclohexanone	293.2	1.13	1.18	4.4%	M.P.	N.A.	[10]
Ethyl Iodide	Ethanol	293.2	6.17	6.09	-1.3%	5.95	-3.6%	[10]
Ethyl Iodide	Ethyl Acetate	293.2	1.55	1.44	-7.1%	1.54	-0.6%	[10]
Ethyl Iodide	Ethyl Acetate	307.2	1.50	1.42	-5.3%	1.52	1.3%	[12]
Ethyl Iodide	Ethyl Acetate	331.7	1.45	1.38	-4.8%	1.48	2.1%	[12]
Ethyl Iodide	Ethyl Acetate	343.9	1.41	1.37	-2.8%	1.46	3.5%	[12]
Ethyl Iodide	Methyl Ethyl Ketone	293.2	1.58	1.48	-6.3%	1.63	3.2%	[10]
Ethyl Iodide	N,N-Dimethylformamide	293.2	2.36	2.58	9.3%	M.P.	N.A.	[10]
Ethyl Iodide	N-Heptane	293.2	1.90	1.89	-0.5%	1.99	4.7%	[10]
Ethyl Iodide	N-Hexane	298.0	2.07	2.02	-2.4%	2.09	1.0%	[12]
Ethyl Iodide	N-Hexane	322.9	1.87	1.85	-1.1%	1.87	0.0%	[12]
Ethyl Iodide	N-Hexane	329.1	1.83	1.81	-1.1%	1.83	0.0%	[12]
Ethyl Iodide	N-Hexane	340.6	1.67	1.75	4.8%	1.75	4.8%	[12]
Ethyl Iodide	Nitrobenzene	293.2	1.83	1.67	-8.7%	M.P.	N.A.	[10]
Ethyl Iodide	Nitroethane	293.2	2.79	2.87	2.9%	2.95	5.7%	[10]
Ethyl Iodide	Nitromethane	293.2	6.16	7.01	13.8%	6.33	2.8%	[10]
Ethyl Iodide	N-Octane	293.2	1.80	1.77	-1.7%	1.86	3.3%	[10]
Ethyl Iodide	Phenol	323.2	2.40	2.51	4.6%	M.P.	N.A.	[10]
Ethyl Iodide	Propionitrile	293.2	2.68	2.67	-0.4%	M.P.	N.A.	[10]
Ethyl Iodide	P-Xylene	293.2	1.03	1.06	2.9%	1.10	6.8%	[10]
Ethyl Iodide	Quinoline	298.2	1.55	1.56	0.6%	M.G.	N.A.	[10]
Ethyl Iodide	Toluene	293.2	1.06	1.02	-3.8%	1.08	1.9%	[10]
Ethylbenzene	1-Octanol	293.4	2.28	2.51	10.1%	2.35	3.1%	[31]
Ethylbenzene	1-Octanol	298.2	2.49	2.46	-1.2%	2.31	-7.2%	[32]
Ethylbenzene	1-Octanol	303.5	2.24	2.42	8.0%	2.27	1.3%	[31]
Ethylbenzene	1-Octanol	313.6	2.15	2.33	8.4%	2.19	1.9%	[31]
Ethylbenzene	1-Octanol	323.4	2.02	2.26	11.9%	2.11	4.5%	[31]
Ethylbenzene	2-Pyrrolidone	303.2	5.64	6.26	11.0%	M.G.	N.A.	[35]
Ethylbenzene	2-Pyrrolidone	313.2	5.60	5.74	2.5%	M.G.	N.A.	[35]
Ethylbenzene	2-Pyrrolidone	323.2	5.56	5.28	-5.0%	M.G.	N.A.	[35]
Ethylbenzene	2-Pyrrolidone	333.2	5.52	4.88	-11.5%	M.G.	N.A.	[35]
Ethylbenzene	Acetonitrile	298.2	5.59	5.93	6.1%	6.36	13.8%	[63]
Ethylbenzene	Acetonitrile	298.2	5.60	5.93	5.9%	6.36	13.6%	[64]
Ethylbenzene	Alpha-Pinene	353.2	1.24	1.22	-1.6%	1.20	-3.2%	[22]
Ethylbenzene	Alpha-Pinene	373.2	1.24	1.20	-3.2%	1.17	-5.6%	[22]
Ethylbenzene	Chlorobenzene	293.2	1.01	1.02	1.0%	1.09	8.0%	39
Ethylbenzene	Ethyl Benzoate	313.2	1.10	1.11	0.9%	M.G.	N.A.	[41]
Ethylbenzene	Ethyl Benzoate	323.2	1.08	1.11	2.8%	M.G.	N.A.	[41]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethylbenzene	Ethyl Benzoate	333.2	1.07	1.10	2.8%	M.G.	N.A.	[41]
Ethylbenzene	Ethyl Benzoate	343.2	1.06	1.10	3.8%	M.G.	N.A.	[41]
Ethylbenzene	Isopropanol	298.2	6.07	5.42	-10.7%	5.10	-16.0%	[63]
Ethylbenzene	Isopropanol	298.2	6.20	5.42	-12.6%	5.10	-17.7%	[64]
Ethylbenzene	Methanol	298.2	13.20	14.10	6.8%	14.22	7.7%	[63]
Ethylbenzene	Methanol	298.2	13.90	14.10	1.4%	14.22	2.3%	[64]
Ethylbenzene	N,N-Dibutylformamide	318.3	1.10	1.09	-1.3%	1.05	-4.9%	[13]
Ethylbenzene	N,N-Dibutylformamide	332.4	1.10	1.08	-1.9%	1.05	-4.6%	[13]
Ethylbenzene	N,N-Dimethylacetamide	303.6	2.07	2.01	-3.0%	1.97	-5.0%	[13]
Ethylbenzene	N,N-Dimethylacetamide	317.6	1.97	1.92	-2.4%	1.93	-1.9%	[13]
Ethylbenzene	N,N-Dimethylacetamide	333.2	1.87	1.83	-2.3%	1.88	0.3%	[13]
Ethylbenzene	N-Formylmorpholine	313.3	3.88	5.00	28.9%	M.G.	N.A.	[43]
Ethylbenzene	N-Formylmorpholine	332.7	3.60	4.32	20.0%	M.G.	N.A.	[43]
Ethylbenzene	N-Formylmorpholine	352.5	3.59	3.79	5.6%	M.G.	N.A.	[43]
Ethylbenzene	N-Formylmorpholine	373.4	3.44	3.36	-2.3%	M.G.	N.A.	[43]
Ethylbenzene	N-Hexadecane	393.2	0.85	0.98	15.3%	0.89	4.7%	[71]
Ethylbenzene	N-Hexadecane	453.2	0.80	0.93	16.3%	0.83	3.7%	[71]
Ethylbenzene	N-Methylacetamide	303.1	5.08	4.93	-2.9%	5.68	11.9%	[13]
Ethylbenzene	N-Methylacetamide	318.4	4.93	4.68	-5.1%	5.55	12.5%	[13]
Ethylbenzene	N-Methylacetamide	331.9	4.82	4.43	-8.1%	5.44	12.9%	[13]
Ethylbenzene	N-Methylformamide	303.2	9.74	9.96	2.2%	M.P.	N.A.	[35]
Ethylbenzene	N-Methylformamide	313.2	9.57	9.29	-2.9%	M.P.	N.A.	[35]
Ethylbenzene	N-Methylformamide	323.2	9.39	8.65	-7.8%	M.P.	N.A.	[35]
Ethylbenzene	N-Methylformamide	333.2	9.23	8.03	-13.0%	M.P.	N.A.	[35]
Ethylbenzene	Propionitrile	313.2	2.36	2.56	8.6%	2.73	15.8%	312
Ethylbenzene	Propionitrile	353.2	2.20	2.12	-3.8%	2.58	17.1%	312
Ethylbenzene	Propionitrile	393.2	2.00	1.85	-7.6%	2.46	22.8%	312
Ethylbenzene	Sulfolane	303.1	5.32	5.71	7.3%	M.G.	N.A.	[13]
Ethylbenzene	Sulfolane	317.9	4.93	4.94	0.2%	M.G.	N.A.	[13]
Ethylbenzene	Sulfolane	332.6	4.44	4.36	-1.7%	M.G.	N.A.	[13]
Ethylbenzene	Tetrahydrofuran	298.2	0.90	0.95	5.6%	0.80	-11.1%	[63]
Ethylbenzene	Tetrahydrofuran	298.2	0.90	0.95	5.6%	0.80	-11.1%	[64]
Ethylbenzene	Tributyl Phosphate	298.6	0.79	0.82	3.8%	M.G.	N.A.	[27]
Ethylbenzene	Tributyl Phosphate	302.9	0.83	0.82	-1.2%	M.G.	N.A.	[27]
Ethylbenzene	Tributyl Phosphate	308.6	0.84	0.82	-2.4%	M.G.	N.A.	[27]
Ethylbenzene	Tributyl Phosphate	313.1	0.84	0.82	-2.4%	M.G.	N.A.	[27]
Ethylbenzene	Tributyl Phosphate	323.7	0.93	0.82	-11.8%	M.G.	N.A.	[27]
Ethylbenzene	Tributyl Phosphate	333.2	0.84	0.81	-3.6%	M.G.	N.A.	[73]
Ethylcyclohexane	1,2-Dichloroethane	298.2	4.94	4.32	-12.6%	3.90	-21.1%	[50]
Ethylcyclohexane	1,4-Dioxane	298.2	6.84	4.53	-33.8%	5.45	-20.3%	[50]
Ethylcyclohexane	1-Butanol	298.2	5.71	6.59	15.4%	5.21	-8.8%	[50]
Ethylcyclohexane	1-Hexene	298.2	1.28	1.07	-16.4%	1.19	-7.0%	[50]
Ethylcyclohexane	1-Octanol	298.2	2.75	3.40	23.6%	2.62	-4.7%	[50]
Ethylcyclohexane	1-Octene	298.2	1.12	1.06	-5.4%	1.14	1.8%	[50]
Ethylcyclohexane	1-Propanol	298.2	7.85	8.41	7.1%	7.32	-6.8%	[50]
Ethylcyclohexane	2,2,4-Trimethylpentane	298.2	1.20	1.33	10.8%	1.05	-12.5%	[50]
Ethylcyclohexane	2-Heptanone	298.2	2.40	2.72	13.3%	2.45	2.1%	[50]
Ethylcyclohexane	2-Pentanone	298.2	3.39	3.71	9.4%	3.49	2.9%	[50]
Ethylcyclohexane	Acetic Acid	298.2	22.64	20.76	-8.3%	20.80	-8.1%	[50]
Ethylcyclohexane	Acetone	298.2	9.35	9.80	4.8%	6.60	-29.4%	[50]
Ethylcyclohexane	Acetonitrile	298.2	41.88	47.01	12.2%	34.01	-18.8%	[50]
Ethylcyclohexane	Acetophenone	298.2	6.11	6.36	4.1%	9.02	47.6%	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethylcyclohexane	Anisole	298.2	3.45	3.53	2.3%	2.86	-17.1%	[50]
Ethylcyclohexane	Benzene	298.2	1.99	1.85	-7.0%	1.78	-10.6%	[50]
Ethylcyclohexane	Benzonitrile	298.2	6.48	7.77	19.9%	M.G.	N.A.	[50]
Ethylcyclohexane	Benzyl Alcohol	298.2	12.88	13.26	3.0%	11.52	-10.6%	[50]
Ethylcyclohexane	Butyl Acetate	298.2	2.42	2.48	2.5%	2.86	18.2%	[50]
Ethylcyclohexane	Butyronitrile	298.2	7.64	8.22	7.6%	8.04	5.2%	[50]
Ethylcyclohexane	Carbon Disulfide	298.2	1.73	1.30	-24.9%	1.35	-22.0%	[50]
Ethylcyclohexane	Carbon Tetrachloride	298.2	1.23	1.17	-4.9%	1.08	-12.2%	[50]
Ethylcyclohexane	Chlorobenzene	298.2	1.98	1.93	-2.5%	1.86	-6.1%	[50]
Ethylcyclohexane	Chloroform	298.2	1.87	2.18	16.6%	1.63	-12.8%	[50]
Ethylcyclohexane	Cyclohexane	298.2	1.05	0.97	-7.6%	1.00	-4.8%	[50]
Ethylcyclohexane	Cyclohexanone	298.2	3.96	4.48	13.1%	2.86	-27.8%	[50]
Ethylcyclohexane	Dichloromethane	298.2	3.39	3.37	-0.6%	3.86	13.9%	[50]
Ethylcyclohexane	Dimethyl Sulfoxide	298.2	83.50	86.91	4.1%	M.P.	N.A.	[50]
Ethylcyclohexane	Ethanol	298.2	13.43	17.12	27.5%	12.52	-6.8%	[50]
Ethylcyclohexane	Ethyl Acetate	298.2	4.30	4.30	0.0%	4.29	-0.2%	[50]
Ethylcyclohexane	Isopropanol	298.2	8.28	9.18	10.9%	6.11	-26.2%	[50]
Ethylcyclohexane	Methanol	298.2	39.07	43.54	11.4%	31.71	-18.8%	[50]
Ethylcyclohexane	Methyl Acetate	298.2	7.43	8.42	13.3%	7.58	2.0%	[50]
Ethylcyclohexane	Methyl Ethyl Ketone	298.2	4.79	5.17	7.9%	4.55	-5.0%	[50]
Ethylcyclohexane	N-Decane	298.2	1.02	0.98	-3.9%	1.01	-1.0%	[50]
Ethylcyclohexane	N-Dodecane	298.2	0.97	0.92	-5.2%	0.98	1.0%	[50]
Ethylcyclohexane	N-Formylmorpholine	313.3	29.60	35.57	20.2%	M.G.	N.A.	[43]
Ethylcyclohexane	N-Formylmorpholine	332.7	23.30	25.59	9.8%	M.G.	N.A.	[43]
Ethylcyclohexane	N-Formylmorpholine	352.5	19.10	19.11	0.1%	M.G.	N.A.	[43]
Ethylcyclohexane	N-Formylmorpholine	373.4	15.50	14.62	-5.7%	M.G.	N.A.	[43]
Ethylcyclohexane	N-Heptane	298.2	1.13	1.08	-4.4%	1.08	-4.4%	[50]
Ethylcyclohexane	N-Hexadecane	298.2	0.85	0.83	-2.4%	0.91	7.1%	[50]
Ethylcyclohexane	N-Hexadecane	298.2	0.84	0.83	-1.2%	0.91	8.3%	[6]
Ethylcyclohexane	N-Hexane	298.2	1.19	1.12	-5.9%	1.11	-6.7%	[50]
Ethylcyclohexane	Nitrobenzene	298.2	8.08	8.08	0.0%	7.27	-10.0%	[50]
Ethylcyclohexane	Nitromethane	298.2	78.93	76.92	-2.5%	74.79	-5.2%	[50]
Ethylcyclohexane	N-Methyl-2-Pyrrolidone	298.2	12.93	12.62	-2.4%	11.06	-14.5%	[50]
Ethylcyclohexane	N-Methylformamide	298.2	45.76	56.11	22.6%	M.P.	N.A.	[50]
Ethylcyclohexane	N-Nonane	298.2	1.03	1.01	-1.9%	1.03	0.0%	[50]
Ethylcyclohexane	N-Octane	298.2	1.01	1.04	3.0%	1.06	5.0%	[50]
Ethylcyclohexane	N-Pentane	298.2	1.40	1.22	-12.9%	1.16	-17.1%	[50]
Ethylcyclohexane	Phenol	328.2	12.28	13.49	9.9%	8.21	-33.1%	[14]
Ethylcyclohexane	Phenol	343.2	10.65	12.13	13.9%	7.44	-30.1%	[14]
Ethylcyclohexane	Phenol	358.2	9.79	10.85	10.8%	6.81	-30.4%	[14]
Ethylcyclohexane	Phenol	373.2	9.04	9.69	7.2%	6.29	-30.4%	[14]
Ethylcyclohexane	Propionitrile	298.2	14.03	15.64	11.5%	9.47	-32.5%	[50]
Ethylcyclohexane	P-Xylene	298.2	1.47	1.42	-3.4%	1.34	-8.8%	[50]
Ethylcyclohexane	Pyridine	298.2	6.04	6.18	2.3%	5.36	-11.3%	[50]
Ethylcyclohexane	Squalane	298.2	0.59	0.72	22.0%	0.72	22.0%	[50]
Ethylcyclohexane	Tetrahydrofuran	298.2	2.14	2.15	0.5%	1.82	-15.0%	[50]
Ethylcyclohexane	Toluene	298.2	1.64	1.62	-1.2%	1.50	-8.5%	[50]
Ethylcyclohexane	Tributyl Phosphate	298.6	1.88	2.43	29.3%	M.G.	N.A.	[27]
Ethylcyclohexane	Tributyl Phosphate	302.9	1.84	2.37	28.8%	M.G.	N.A.	[27]
Ethylcyclohexane	Tributyl Phosphate	308.6	1.79	2.29	27.9%	M.G.	N.A.	[27]
Ethylcyclohexane	Tributyl Phosphate	313.1	1.77	2.24	26.6%	M.G.	N.A.	[27]
Ethylcyclohexane	Triethylamine	298.2	1.09	1.29	18.3%	M.P.	N.A.	[50]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Ethylene Glycol Ethyl Ether	1-Propanol	313.2	1.23	1.41	14.4%	0.95	-22.9%	383
Ethylene Glycol Ethyl Ether	Di-N-Propyl Ether	313.2	4.74	5.10	7.6%	6.29	32.7%	348
Ethylene Glycol Ethyl Ether	Di-N-Propyl Ether	323.2	4.36	4.53	3.8%	5.84	33.8%	348
Ethylene Glycol Ethyl Ether	Di-N-Propyl Ether	333.2	3.99	4.08	2.3%	5.42	35.9%	348
Ethylene Glycol Ethyl Ether	Ethanol	313.2	1.16	1.19	2.5%	0.89	-23.3%	383
Ethylene Glycol Ethyl Ether	Ethyl Acetate	313.2	2.13	2.85	33.6%	2.25	5.5%	391
Ethylene Glycol Ethyl Ether	Isopropanol	313.2	1.20	1.71	42.1%	0.96	-20.2%	383
Ethylene Glycol Ethyl Ether	Methanol	313.2	0.99	0.74	-25.5%	0.66	-33.5%	383
Ethylene Glycol Ethyl Ether	Methyl Acetate	313.2	2.18	2.24	2.9%	3.51	61.2%	391
Ethylene Glycol Ethyl Ether	Methyl Formate	308.2	2.52	2.97	17.6%	M.P.	N.A.	391
Ethylene Glycol Ethyl Ether	Phenol	363.2	0.07	0.11	65.2%	0.10	50.2%	398
Ethylene Glycol Ethyl Ether	Phenol	373.2	0.09	0.11	29.3%	0.11	29.3%	398
Ethylene Glycol Ethyl Ether	Phenol	383.2	0.11	0.12	9.0%	0.12	9.0%	398
Ethylene Glycol Ethyl Ether	Propyl Acetate	313.2	2.20	3.00	36.3%	1.35	-38.6%	391
Isopentane	Acetonitrile	293.2	26.33	21.79	-17.2%	11.24	-57.3%	[45]
Isopentane	Acetonitrile	313.2	20.86	15.17	-27.3%	8.47	-59.4%	[45]
Isopentane	Acetonitrile	333.2	16.50	11.16	-32.4%	6.58	-60.1%	[45]
Isopentane	Aniline	293.2	20.29	20.32	0.1%	8.72	-57.0%	[37]
Isopentane	N-Methylformamide	303.2	30.48	32.12	5.4%	M.P.	N.A.	[35]
Isopentane	N-Methylformamide	313.2	28.08	28.69	2.2%	M.P.	N.A.	[35]
Isopentane	N-Methylformamide	323.2	25.58	25.60	0.1%	M.P.	N.A.	[35]
Isopentane	N-Methylformamide	333.2	23.84	22.86	-4.1%	M.P.	N.A.	[35]
Isopentane	Quinoline	293.2	8.53	8.09	-5.2%	M.G.	N.A.	[37]
Isopropanol	1,4-Dioxane	323.2	2.36	2.44	3.4%	2.03	-14.0%	330
Isopropanol	1,4-Dioxane	333.2	2.12	2.33	9.8%	1.91	-10.0%	330
Isopropanol	1,4-Dioxane	343.2	2.01	2.25	11.8%	1.81	-10.1%	330
Isopropanol	1,4-Dioxane	353.2	1.69	2.17	28.3%	1.71	1.1%	330
Isopropanol	1-Butanol	313.2	0.98	1.02	4.3%	1.01	3.3%	13
Isopropanol	1-Octanol	293.4	1.05	1.14	8.6%	1.07	1.9%	[31]
Isopropanol	1-Octanol	298.2	1.12	1.13	0.9%	1.07	-4.5%	[3]
Isopropanol	1-Octanol	303.5	1.08	1.12	3.7%	1.07	-0.9%	[31]
Isopropanol	1-Octanol	313.6	1.05	1.11	5.7%	1.07	1.9%	[31]
Isopropanol	1-Octanol	323.4	1.02	1.10	7.8%	1.06	3.9%	[31]
Isopropanol	1-Phenyl-1-Butanone	298.1	4.83	3.96	-18.0%	3.21	-33.5%	[34]
Isopropanol	2,6-Dimethylpyridine	313.2	1.10	0.95	-13.9%	1.53	38.7%	167
Isopropanol	2-Methyl-1-Propanol	313.2	0.97	1.01	3.7%	1.01	3.7%	12
Isopropanol	Benzene	313.2	13.90	10.45	-24.8%	10.20	-26.6%	325
Isopropanol	Butyronitrile	278.2	4.93	4.30	-12.9%	1.46	-70.4%	28
Isopropanol	Butyronitrile	288.2	4.08	3.91	-4.1%	1.46	-64.2%	28
Isopropanol	Butyronitrile	293.2	3.77	3.74	-0.9%	1.44	-61.8%	28
Isopropanol	Butyronitrile	298.2	3.49	3.58	2.6%	1.42	-59.3%	28
Isopropanol	Butyronitrile	303.2	3.29	3.44	4.6%	1.40	-57.4%	28
Isopropanol	Butyronitrile	308.2	3.11	3.31	6.5%	1.37	-55.9%	28

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Isopropanol	Butyronitrile	313.2	2.91	3.19	9.7%	1.34	-53.9%	28
Isopropanol	Butyronitrile	323.2	2.73	2.99	9.6%	1.28	-53.1%	28
Isopropanol	Chloroform	323.2	2.91	2.99	2.6%	3.89	33.5%	234
Isopropanol	Cyclohexane	312.9	23.40	25.01	6.9%	30.44	30.1%	[17]
Isopropanol	Cyclohexane	313.2	28.00	24.81	-11.4%	30.17	7.8%	[21]
Isopropanol	Cyclohexane	322.9	18.34	19.62	7.0%	22.89	24.8%	[17]
Isopropanol	Cyclohexane	323.2	17.05	19.49	14.3%	22.70	33.1%	228
Isopropanol	Cyclohexane	333.0	15.72	15.75	0.2%	17.44	10.9%	[17]
Isopropanol	Cyclohexane	333.2	13.72	15.69	14.4%	17.35	26.5%	228
Isopropanol	Cyclohexane	333.2	13.65	15.69	14.9%	17.35	27.1%	[21]
Isopropanol	Cyclohexane	343.0	12.74	12.96	1.7%	13.55	6.4%	[17]
Isopropanol	Cyclohexane	352.9	10.45	10.88	4.1%	10.72	2.6%	[17]
Isopropanol	Diethyl Phthalate	303.2	2.83	2.70	-4.6%	2.24	-20.8%	[39]
Isopropanol	Diethyl Phthalate	313.2	2.57	2.51	-2.3%	2.04	-20.6%	[39]
Isopropanol	Diethyl Phthalate	323.2	2.38	2.35	-1.3%	1.88	-21.0%	[39]
Isopropanol	Diethyl Phthalate	333.2	2.17	2.21	1.8%	1.74	-19.8%	[39]
Isopropanol	Di-N-Propyl Ether	278.2	6.42	8.02	25.0%	4.68	-27.0%	451
Isopropanol	Di-N-Propyl Ether	288.2	6.07	6.72	10.8%	4.30	-29.1%	451
Isopropanol	Di-N-Propyl Ether	293.2	5.81	6.19	6.5%	4.13	-28.9%	451
Isopropanol	Di-N-Propyl Ether	298.2	5.60	5.74	2.6%	3.97	-29.1%	451
Isopropanol	Di-N-Propyl Ether	303.2	5.36	5.34	-0.4%	3.83	-28.5%	451
Isopropanol	Di-N-Propyl Ether	308.2	5.07	4.99	-1.7%	3.69	-27.3%	451
Isopropanol	Di-N-Propyl Ether	313.2	4.81	4.67	-2.9%	3.56	-26.0%	451
Isopropanol	Di-N-Propyl Ether	323.2	4.27	4.15	-2.9%	3.33	-22.1%	451
Isopropanol	Epsilon-Caprolactone	303.2	2.18	2.37	8.7%	M.G.	N.A.	[41]
Isopropanol	Epsilon-Caprolactone	318.2	1.99	2.24	12.6%	M.G.	N.A.	[41]
Isopropanol	Epsilon-Caprolactone	333.2	1.83	2.13	16.4%	M.G.	N.A.	[41]
Isopropanol	Ethyl Acetate	288.2	4.63	4.13	-10.8%	2.63	-43.2%	[79]
Isopropanol	Ethyl Acetate	328.2	2.19	2.89	32.3%	1.84	-15.8%	236
Isopropanol	Ethylene Glycol Ethyl Ether	313.2	1.13	1.26	11.3%	0.97	-14.3%	383
Isopropanol	Glutaronitrile	303.2	5.26	5.49	4.4%	9.14	73.8%	[39]
Isopropanol	Glutaronitrile	313.2	4.68	5.01	7.1%	8.24	76.1%	[39]
Isopropanol	Glutaronitrile	323.2	4.26	4.60	8.0%	7.47	75.4%	[39]
Isopropanol	Glutaronitrile	333.2	3.85	4.26	10.6%	6.82	77.1%	[39]
Isopropanol	Methyl Ethyl Ketone	278.2	2.73	2.73	0.1%	2.51	-8.0%	262
Isopropanol	Methyl Ethyl Ketone	288.2	2.51	2.56	2.0%	2.30	-8.3%	262
Isopropanol	Methyl Ethyl Ketone	293.2	2.36	2.48	5.2%	2.22	-5.8%	262
Isopropanol	Methyl Ethyl Ketone	298.2	2.28	2.41	5.9%	2.13	-6.4%	262
Isopropanol	Methyl Ethyl Ketone	308.2	2.08	2.28	9.6%	1.99	-4.3%	262
Isopropanol	Methyl Ethyl Ketone	313.2	2.02	2.22	9.9%	1.92	-4.9%	262
Isopropanol	Methyl Ethyl Ketone	323.2	1.87	2.12	13.5%	1.81	-3.1%	262
Isopropanol	N,N-Dibutylformamide	318.3	0.81	0.78	-4.2%	1.02	25.3%	[13]
Isopropanol	N,N-Dibutylformamide	332.5	0.80	0.79	-0.8%	1.00	25.6%	[13]
Isopropanol	N,N-Diethylacetamide	303.2	0.54	0.47	-13.1%	0.76	40.5%	[39]
Isopropanol	N,N-Diethylacetamide	313.2	0.54	0.50	-7.9%	0.76	40.0%	[39]
Isopropanol	N,N-Diethylacetamide	323.2	0.54	0.53	-2.4%	0.77	41.8%	[39]
Isopropanol	N,N-Diethylacetamide	333.2	0.54	0.55	1.3%	0.77	41.8%	[39]
Isopropanol	N,N-Dimethylacetamide	303.2	0.60	0.60	-0.5%	0.65	7.8%	[13]
Isopropanol	N,N-Dimethylacetamide	317.6	0.58	0.65	12.5%	0.65	12.5%	[13]
Isopropanol	N,N-Dimethylacetamide	333.2	0.55	0.71	28.2%	0.65	17.3%	[13]
Isopropanol	N,N-Dimethylformamide	353.2	0.88	0.96	8.7%	0.76	-14.0%	276
Isopropanol	N-Ethylacetamide	303.2	0.85	0.82	-3.3%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Isopropanol	N-Ethylacetamide	313.2	0.84	0.82	-2.6%	M.G.	N.A.	[39]
Isopropanol	N-Ethylacetamide	323.2	0.84	0.82	-2.3%	M.G.	N.A.	[39]
Isopropanol	N-Ethylacetamide	333.2	0.84	0.82	-1.8%	M.G.	N.A.	[39]
Isopropanol	N-Formylmorpholine	303.5	1.94	2.04	5.2%	M.G.	N.A.	[43]
Isopropanol	N-Formylmorpholine	323.2	1.70	1.90	11.8%	M.G.	N.A.	[43]
Isopropanol	N-Formylmorpholine	342.8	1.52	1.80	18.4%	M.G.	N.A.	[43]
Isopropanol	N-Heptane	303.2	25.16	25.28	0.5%	28.00	11.3%	308
Isopropanol	N-Hexadecane	298.2	26.52	25.63	-3.4%	21.53	-18.8%	[6]
Isopropanol	N-Hexane	318.4	18.80	17.21	-8.5%	20.94	11.4%	[17]
Isopropanol	N-Hexane	328.2	12.29	13.81	12.4%	16.82	36.9%	224
Isopropanol	N-Hexane	328.4	14.88	13.77	-7.5%	16.77	12.7%	[17]
Isopropanol	N-Hexane	341.4	11.35	10.65	-6.2%	12.79	12.7%	[17]
Isopropanol	N-Methyl-2-Pyrrolidone	323.4	0.75	0.56	-25.7%	0.59	-21.8%	[43]
Isopropanol	N-Methyl-2-Pyrrolidone	333.2	0.76	0.60	-20.5%	0.53	-29.8%	[43]
Isopropanol	N-Methyl-2-Pyrrolidone	343.4	0.74	0.64	-13.2%	0.48	-34.9%	[43]
Isopropanol	N-Methylacetamide	303.2	0.99	1.03	3.8%	1.06	6.9%	[13]
Isopropanol	N-Methylacetamide	318.4	0.96	1.01	5.3%	1.03	7.4%	[13]
Isopropanol	N-Methylacetamide	333.3	0.93	1.01	8.1%	1.03	10.3%	[13]
Isopropanol	N-Octane	353.2	7.40	8.41	13.6%	8.86	19.7%	225
Isopropanol	Pyridine	313.2	1.23	1.12	-8.8%	0.85	-30.8%	183
Isopropanol	Sulfolane	303.8	4.35	4.18	-3.8%	M.G.	N.A.	[13]
Isopropanol	Sulfolane	317.9	3.60	3.78	4.9%	M.G.	N.A.	[13]
Isopropanol	Sulfolane	332.8	2.86	3.45	20.5%	M.G.	N.A.	[13]
Isopropanol	Tetraethylene Glycol DME	303.2	1.40	1.03	-26.2%	0.99	-29.1%	[7]
Isopropanol	Tetraethylene Glycol DME	323.2	1.24	1.01	-18.6%	0.89	-28.3%	[7]
Isopropanol	Tetraethylene Glycol DME	343.2	1.10	1.00	-8.9%	0.84	-23.5%	[7]
Isopropanol	Toluene	293.2	13.52	15.56	15.1%	15.19	12.4%	[33]
Isopropanol	Toluene	293.2	13.24	15.56	17.5%	15.19	14.7%	[33]
Isopropanol	Toluene	303.2	11.28	12.55	11.3%	11.76	4.3%	[33]
Isopropanol	Toluene	313.2	10.51	10.36	-1.4%	9.36	-10.9%	[33]
M-Cresol	Aniline	407.9	0.76	0.70	-7.5%	0.77	1.8%	282
M-Cresol	Aniline	407.9	0.75	0.70	-6.7%	0.77	2.7%	[61]
M-Cresol	Aniline	408.2	0.76	0.70	-7.9%	0.77	1.3%	[61]
M-Cresol	Aniline	422.9	0.77	0.72	-7.1%	0.80	3.2%	282
M-Cresol	Aniline	422.9	0.77	0.72	-6.5%	0.80	3.9%	[61]
M-Cresol	Aniline	437.9	0.77	0.74	-4.5%	0.81	4.5%	282
M-Cresol	Aniline	437.9	0.80	0.74	-7.5%	0.81	1.3%	[61]
M-Cresol	Aniline	453.2	0.82	0.76	-6.9%	0.82	0.5%	282
M-Cresol	Aniline	453.2	0.78	0.76	-2.6%	0.82	5.1%	[61]
Methanol	1,2-Dichloroethane	318.4	9.10	8.45	-7.1%	7.76	-14.7%	[12]
Methanol	1,2-Dichloroethane	323.2	9.97	7.84	-21.3%	7.16	-28.2%	314
Methanol	1,2-Dichloroethane	337.2	6.93	6.42	-7.4%	5.72	-17.5%	[12]
Methanol	1,2-Dichloroethane	355.0	5.50	5.15	-6.4%	4.41	-19.8%	[12]
Methanol	1-Butanol	308.2	1.12	1.18	5.4%	1.14	1.8%	[30]
Methanol	1-Butanol	313.2	1.11	1.17	5.1%	1.13	1.5%	5
Methanol	1-Butanol	318.2	1.08	1.16	7.4%	1.12	3.7%	[30]
Methanol	1-Butanol	328.2	1.05	1.15	9.5%	1.11	5.7%	[30]
Methanol	1-Octanol	293.4	1.25	1.69	35.2%	1.39	11.2%	[31]
Methanol	1-Octanol	298.2	1.34	1.66	23.9%	1.38	3.0%	[3]
Methanol	1-Octanol	303.5	1.25	1.63	30.4%	1.36	8.8%	[31]
Methanol	1-Octanol	313.6	1.25	1.56	24.8%	1.33	6.4%	[31]
Methanol	1-Octanol	323.4	1.19	1.50	26.1%	1.31	10.1%	[31]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methanol	1-Pentanol	303.5	1.15	1.32	14.8%	1.21	5.2%	[33]
Methanol	1-Pentanol	308.2	1.24	1.30	4.8%	1.20	-3.2%	[30]
Methanol	1-Pentanol	313.2	1.12	1.29	15.2%	1.19	6.2%	[33]
Methanol	1-Pentanol	318.2	1.35	1.28	-5.2%	1.18	-12.6%	[30]
Methanol	1-Pentanol	323.5	1.13	1.27	12.4%	1.17	3.5%	[33]
Methanol	1-Pentanol	328.2	1.20	1.26	5.0%	1.16	-3.3%	[30]
Methanol	1-Phenyl-1-Butanone	298.1	4.32	5.16	19.4%	3.08	-28.7%	[34]
Methanol	1-Propanol	313.2	1.06	1.16	9.9%	1.07	1.4%	7
Methanol	1-Propanol	333.2	1.05	1.14	8.4%	1.05	-0.1%	7
Methanol	2,2,4-Trimethylpentane	293.2	78.00	77.03	-1.2%	79.44	1.8%	[10]
Methanol	2,6-Dimethylpyridine	313.2	0.74	1.25	68.4%	2.90	290.7%	170
Methanol	2-Methyl-1-Propanol	313.2	1.07	1.20	11.7%	1.13	5.2%	17
Methanol	2-Methyl-2-Propanol	313.2	0.60	1.14	88.7%	1.28	111.8%	11
Methanol	2-Nitropropane	293.2	8.35	8.18	-2.0%	7.11	-14.9%	[10]
Methanol	2-Pyrrolidone	303.2	0.74	0.65	-12.6%	M.G.	N.A.	[35]
Methanol	2-Pyrrolidone	313.2	0.75	0.65	-13.6%	M.G.	N.A.	[35]
Methanol	2-Pyrrolidone	323.2	0.76	0.66	-13.0%	M.G.	N.A.	[35]
Methanol	2-Pyrrolidone	333.2	0.77	0.66	-13.8%	M.G.	N.A.	[35]
Methanol	Acetone	303.2	2.11	2.08	-1.4%	2.05	-2.8%	[18]
Methanol	Acetone	308.3	1.99	2.02	1.5%	2.00	0.5%	[18]
Methanol	Acetone	313.3	1.93	1.96	1.6%	1.95	1.0%	[18]
Methanol	Acetone	323.2	1.91	1.87	-2.0%	1.87	-2.0%	214
Methanol	Acetone	329.3	1.71	1.82	6.4%	1.82	6.4%	[59]
Methanol	Acetone	329.4	1.77	1.82	2.8%	1.82	2.8%	[11]
Methanol	Acetone	329.4	1.75	1.82	4.0%	1.82	4.0%	[11]
Methanol	Acetonitrile	326.0	2.56	2.18	-14.9%	2.54	-0.8%	207
Methanol	Acetonitrile	333.5	2.54	2.11	-16.9%	2.42	-4.7%	207
Methanol	Acetophenone	293.2	3.47	3.85	11.0%	2.92	-15.9%	[10]
Methanol	Aniline	293.2	2.39	2.31	-3.3%	2.25	-5.9%	[10]
Methanol	Anisole	293.2	11.00	12.04	9.5%	4.59	-58.3%	[10]
Methanol	Benzene	298.2	19.40	21.97	13.2%	21.05	8.5%	[46]
Methanol	Benzonitrile	293.2	4.70	5.05	7.4%	M.G.	N.A.	[10]
Methanol	Butyronitrile	278.2	4.01	4.13	3.0%	1.06	-73.6%	31
Methanol	Butyronitrile	288.2	3.76	3.67	-2.4%	1.05	-72.1%	31
Methanol	Butyronitrile	298.2	3.42	3.31	-3.1%	1.04	-69.6%	31
Methanol	Butyronitrile	308.2	3.18	3.01	-5.3%	1.02	-67.9%	31
Methanol	Butyronitrile	318.2	2.92	2.77	-5.2%	0.99	-66.1%	31
Methanol	Carbon Tetrachloride	293.2	48.30	43.28	-10.4%	54.86	13.6%	[28]
Methanol	Carbon Tetrachloride	313.2	26.40	23.74	-10.1%	34.81	31.9%	[28]
Methanol	Carbon Tetrachloride	333.2	13.10	14.68	12.1%	23.33	78.1%	[28]
Methanol	Chlorobenzene	328.2	14.14	11.44	-19.1%	13.86	-2.0%	132
Methanol	Chloroform	293.2	8.43	11.75	39.4%	13.07	55.0%	261
Methanol	Chloroform	298.2	9.55	10.59	10.9%	11.77	23.2%	[30]
Methanol	Chloroform	303.2	8.09	9.60	18.7%	10.68	32.0%	261
Methanol	Chloroform	316.0	6.38	7.65	19.9%	8.59	34.6%	[12]
Methanol	Chloroform	318.2	9.71	7.38	-24.0%	8.31	-14.4%	[60]
Methanol	Chloroform	323.2	8.66	6.82	-21.2%	7.74	-10.6%	261
Methanol	Chloroform	328.2	9.24	6.33	-31.5%	7.25	-21.5%	[60]
Methanol	Chloroform	328.4	6.93	6.31	-8.9%	7.23	4.3%	[12]
Methanol	Cyclohexane	283.2	118.80	134.54	13.2%	112.62	-5.2%	[79]
Methanol	Cyclohexane	293.2	77.80	88.02	13.1%	82.26	5.7%	[79]
Methanol	Cyclohexane	308.2	54.20	50.81	-6.3%	53.35	-1.6%	[76]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methanol	Cyclohexane	313.2	63.70	43.16	-32.2%	46.61	-26.8%	[79]
Methanol	Cyclohexane	318.2	38.00	36.98	-2.7%	40.89	7.6%	[76]
Methanol	Cyclohexane	333.2	27.50	24.39	-11.3%	28.26	2.8%	[76]
Methanol	Cyclopentane	288.2	168.50	107.82	-36.0%	105.33	-37.5%	[79]
Methanol	Dichloromethane	298.2	15.88	9.77	-38.5%	16.33	2.8%	220
Methanol	Dichloromethane	348.2	6.97	4.86	-30.3%	7.04	1.0%	220
Methanol	Dichloromethane	398.2	3.90	3.13	-19.7%	3.74	-4.1%	220
Methanol	Diethyl Ether	298.2	4.72	7.96	68.6%	5.64	19.4%	150
Methanol	Diethyl Ether	338.2	3.82	4.30	12.6%	4.55	19.1%	150
Methanol	Diethyl Ether	388.2	2.88	2.63	-8.5%	3.44	19.6%	150
Methanol	Diethyl Phthalate	303.2	2.54	3.06	20.5%	2.76	8.7%	[39]
Methanol	Diethyl Phthalate	313.2	2.35	2.76	17.4%	2.59	10.2%	[39]
Methanol	Diethyl Phthalate	323.2	2.21	2.50	13.1%	2.43	10.0%	[39]
Methanol	Diethyl Phthalate	333.2	2.06	2.29	11.2%	2.28	10.7%	[39]
Methanol	Dimethyl Carbonate	313.2	4.03	4.21	4.6%	M.G.	N.A.	251
Methanol	Di-N-Propyl Ether	278.2	8.11	14.77	82.2%	7.62	-6.0%	74
Methanol	Di-N-Propyl Ether	288.2	7.80	11.58	48.5%	7.15	-8.3%	74
Methanol	Di-N-Propyl Ether	293.2	7.49	10.36	38.4%	6.93	-7.4%	74
Methanol	Di-N-Propyl Ether	298.2	7.11	9.32	31.1%	6.71	-5.6%	74
Methanol	Di-N-Propyl Ether	303.2	6.87	8.43	22.7%	6.50	-5.4%	74
Methanol	Di-N-Propyl Ether	308.2	6.74	7.67	13.8%	6.29	-6.7%	74
Methanol	Di-N-Propyl Ether	313.2	6.38	7.01	9.9%	6.09	-4.5%	74
Methanol	Di-N-Propyl Ether	323.2	5.93	5.93	0.1%	5.70	-3.8%	74
Methanol	Epsilon-Caprolactone	303.2	1.65	1.63	-1.2%	M.G.	N.A.	[41]
Methanol	Epsilon-Caprolactone	318.2	1.56	1.54	-1.3%	M.G.	N.A.	[41]
Methanol	Epsilon-Caprolactone	333.2	1.44	1.46	1.4%	M.G.	N.A.	[41]
Methanol	Ethyl Acetate	350.4	2.65	2.78	4.9%	2.59	-2.3%	[12]
Methanol	Ethylene Glycol Ethyl Ether	313.2	0.99	0.91	-8.4%	0.85	-14.5%	383
Methanol	Glutaronitrile	303.2	2.85	2.53	-11.2%	2.80	-1.8%	[39]
Methanol	Glutaronitrile	313.2	2.63	2.39	-9.1%	2.61	-0.8%	[39]
Methanol	Glutaronitrile	323.2	2.45	2.26	-7.8%	2.44	-0.4%	[39]
Methanol	Glutaronitrile	333.2	2.27	2.14	-5.7%	2.29	0.9%	[39]
Methanol	Methyl Ethyl Ketone	288.2	2.56	3.02	18.2%	2.30	-10.0%	263
Methanol	Methyl Ethyl Ketone	298.2	2.45	2.75	12.4%	2.19	-10.5%	263
Methanol	Methyl Ethyl Ketone	303.2	2.37	2.64	11.4%	2.14	-9.7%	263
Methanol	Methyl Ethyl Ketone	303.2	2.42	2.64	9.1%	2.14	-11.6%	[18]
Methanol	Methyl Ethyl Ketone	308.2	2.32	2.53	9.1%	2.09	-9.9%	263
Methanol	Methyl Ethyl Ketone	313.0	2.24	2.44	8.9%	2.05	-8.5%	[18]
Methanol	Methyl Ethyl Ketone	313.2	2.26	2.44	7.8%	2.05	-9.5%	263
Methanol	Methyl Ethyl Ketone	313.2	2.22	2.44	9.9%	2.05	-7.7%	[18]
Methanol	Methyl Ethyl Ketone	314.7	2.29	2.41	5.2%	2.03	-11.4%	[12]
Methanol	Methyl Ethyl Ketone	323.2	2.20	2.27	3.2%	1.96	-10.9%	263
Methanol	Methyl Ethyl Ketone	333.1	2.16	2.13	-1.4%	1.88	-13.0%	[18]
Methanol	Methyl Ethyl Ketone	333.3	2.09	2.13	1.9%	1.88	-10.0%	[12]
Methanol	N,N-Dibutylformamide	302.8	0.79	1.02	29.9%	1.27	61.8%	[13]
Methanol	N,N-Dibutylformamide	318.3	0.78	0.98	25.2%	1.30	66.0%	[13]
Methanol	N,N-Dibutylformamide	332.4	0.79	0.94	18.8%	1.30	64.3%	[13]
Methanol	N,N-Diethylacetamide	303.2	0.42	0.49	17.2%	0.73	74.6%	[39]
Methanol	N,N-Diethylacetamide	313.2	0.43	0.50	15.2%	0.75	72.8%	[39]
Methanol	N,N-Diethylacetamide	323.2	0.45	0.52	16.6%	0.77	72.6%	[39]
Methanol	N,N-Diethylacetamide	333.2	0.46	0.54	17.4%	0.79	71.7%	[39]
Methanol	N,N-Dimethylacetamide	303.6	0.42	0.45	6.6%	0.43	1.9%	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methanol	N,N-Dimethylacetamide	317.6	0.44	0.49	12.6%	0.45	3.4%	[13]
Methanol	N,N-Dimethylacetamide	333.4	0.46	0.53	14.5%	0.47	1.5%	[13]
Methanol	N,N-Dimethylformamide	313.2	0.64	0.57	-10.6%	0.67	5.1%	65
Methanol	N-Decane	293.2	84.10	77.22	-8.2%	69.42	-17.5%	[23]
Methanol	N-Dodecane	293.2	80.00	76.61	-4.2%	62.04	-22.5%	[23]
Methanol	N-Ethylacetamide	303.2	0.66	0.61	-7.7%	M.G.	N.A.	[39]
Methanol	N-Ethylacetamide	313.2	0.66	0.61	-8.1%	M.G.	N.A.	[39]
Methanol	N-Ethylacetamide	323.2	0.67	0.61	-9.1%	M.G.	N.A.	[39]
Methanol	N-Ethylacetamide	333.2	0.67	0.61	-9.4%	M.G.	N.A.	[39]
Methanol	N-Formylmorpholine	303.5	1.07	0.99	-7.5%	M.G.	N.A.	[43]
Methanol	N-Formylmorpholine	323.2	1.05	0.97	-7.6%	M.G.	N.A.	[43]
Methanol	N-Formylmorpholine	342.8	1.04	0.95	-8.7%	M.G.	N.A.	[43]
Methanol	N-Heptane	288.2	115.80	96.90	-16.3%	99.75	-13.9%	[23]
Methanol	N-Heptane	293.2	80.00	78.77	-1.5%	86.05	7.6%	[10]
Methanol	N-Heptane	293.2	97.50	78.77	-19.2%	86.05	-11.7%	[23]
Methanol	N-Heptane	298.2	81.80	64.79	-20.8%	74.60	-8.8%	[23]
Methanol	N-Heptane	303.2	71.40	53.88	-24.5%	64.98	-9.0%	[23]
Methanol	N-Heptane	308.2	60.70	45.26	-25.4%	56.86	-6.3%	[23]
Methanol	N-Heptane	313.2	51.90	38.39	-26.0%	49.96	-3.7%	[18]
Methanol	N-Heptane	313.2	53.80	38.39	-28.6%	49.96	-7.1%	[23]
Methanol	N-Heptane	318.2	46.50	32.85	-29.4%	44.07	-5.2%	[23]
Methanol	N-Heptane	323.2	38.50	28.34	-26.4%	39.03	1.4%	[18]
Methanol	N-Heptane	323.2	40.80	28.34	-30.5%	39.03	-4.3%	[23]
Methanol	N-Heptane	333.2	28.00	21.57	-23.0%	30.95	10.5%	[18]
Methanol	N-Hexadecane	293.2	69.90	74.47	6.5%	51.74	-26.0%	[23]
Methanol	N-Hexadecane	298.2	52.91	60.71	14.7%	44.86	-15.2%	[6]
Methanol	N-Hexane	288.2	125.50	97.43	-22.4%	109.32	-12.9%	[23]
Methanol	N-Hexane	293.2	104.00	79.29	-23.8%	94.31	-9.3%	[23]
Methanol	N-Hexane	298.2	90.50	65.30	-27.8%	81.77	-9.6%	[23]
Methanol	N-Hexane	303.2	78.20	54.37	-30.5%	71.22	-8.9%	[23]
Methanol	N-Hexane	308.2	67.80	45.73	-32.6%	62.31	-8.1%	[23]
Methanol	N-Hexane	313.2	55.80	38.83	-30.4%	54.75	-1.9%	[18]
Methanol	N-Hexane	313.2	58.30	38.83	-33.4%	54.75	-6.1%	[23]
Methanol	N-Hexane	318.2	50.70	33.26	-34.4%	48.30	-4.7%	[23]
Methanol	N-Hexane	333.3	39.10	21.86	-44.1%	33.84	-13.5%	[18]
Methanol	N-Hexane	341.3	34.40	17.95	-47.8%	28.39	-17.5%	[17]
Methanol	Nitrobenzene	293.2	10.40	10.44	0.4%	M.P.	N.A.	[10]
Methanol	Nitroethane	293.2	6.07	5.87	-3.3%	6.78	11.7%	[10]
Methanol	Nitromethane	298.2	7.24	4.98	-31.2%	6.44	-11.1%	195
Methanol	Nitromethane	348.2	4.01	3.21	-19.9%	3.87	-3.4%	195
Methanol	Nitromethane	388.2	2.83	2.53	-10.7%	2.95	4.2%	195
Methanol	N-Methyl-2-Pyrrolidone	323.4	0.53	0.36	-31.7%	M.P.	N.A.	[43]
Methanol	N-Methyl-2-Pyrrolidone	333.2	0.52	0.39	-25.1%	M.P.	N.A.	[43]
Methanol	N-Methyl-2-Pyrrolidone	343.4	0.52	0.42	-18.8%	M.P.	N.A.	[43]
Methanol	N-Methylacetamide	303.2	0.70	0.65	-6.6%	0.64	-8.0%	[13]
Methanol	N-Methylacetamide	318.4	0.71	0.65	-7.8%	0.66	-6.4%	[13]
Methanol	N-Methylacetamide	332.8	0.72	0.65	-9.1%	0.67	-6.3%	[13]
Methanol	N-Methylacetamide	398.6	0.70	0.69	-1.9%	0.70	-0.4%	328
Methanol	N-Methylformamide	303.2	1.04	0.91	-12.6%	M.P.	N.A.	255
Methanol	N-Methylformamide	303.2	1.06	0.91	-14.3%	M.P.	N.A.	[35]
Methanol	N-Methylformamide	313.2	1.20	0.90	-24.8%	M.P.	N.A.	255
Methanol	N-Methylformamide	313.2	1.03	0.90	-12.7%	M.P.	N.A.	[35]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methanol	N-Methylformamide	323.2	0.99	0.90	-9.5%	M.P.	N.A.	[35]
Methanol	N-Methylformamide	333.2	0.97	0.90	-7.1%	M.P.	N.A.	[35]
Methanol	N-Octane	288.2	112.90	96.34	-14.7%	92.10	-18.4%	[23]
Methanol	N-Octane	293.2	80.00	78.21	-2.2%	79.45	-0.7%	[10]
Methanol	N-Octane	293.2	95.10	78.21	-17.8%	79.45	-16.5%	[23]
Methanol	N-Octane	298.2	84.00	64.25	-23.5%	68.88	-18.0%	[23]
Methanol	N-Octane	303.2	72.30	53.37	-26.2%	60.00	-17.0%	[23]
Methanol	N-Octane	308.2	60.00	44.78	-25.4%	52.50	-12.5%	[23]
Methanol	N-Octane	313.2	54.00	37.94	-29.7%	46.13	-14.6%	[23]
Methanol	N-Octane	318.2	46.80	32.42	-30.7%	40.69	-13.1%	[23]
Methanol	N-Octane	323.2	40.70	27.94	-31.4%	36.04	-11.4%	[23]
Methanol	N-Tetradecane	293.2	74.70	75.47	1.0%	56.33	-24.6%	[23]
Methanol	P-Xylene	313.2	20.01	18.82	-5.9%	15.45	-22.8%	46
Methanol	Pyridine	298.2	0.87	1.03	17.9%	0.76	-13.0%	257
Methanol	Pyridine	308.2	0.90	1.02	12.8%	0.78	-13.7%	257
Methanol	Pyridine	313.2	1.26	1.02	-19.3%	0.79	-37.5%	257
Methanol	Pyridine	318.2	0.93	1.02	9.5%	0.80	-14.1%	257
Methanol	Sulfolane	303.8	2.34	1.89	-19.1%	M.G.	N.A.	[13]
Methanol	Sulfolane	317.9	2.08	1.78	-14.5%	M.G.	N.A.	[13]
Methanol	Sulfolane	333.7	1.87	1.67	-10.6%	M.G.	N.A.	[13]
Methanol	Tetraethylene Glycol DME	303.2	0.94	1.17	24.2%	1.00	6.2%	[7]
Methanol	Tetraethylene Glycol DME	323.2	0.87	1.08	23.7%	0.94	7.7%	[7]
Methanol	Tetraethylene Glycol DME	343.2	0.80	1.00	25.0%	0.88	10.0%	[7]
Methanol	Toluene	293.2	22.07	27.59	25.0%	20.98	-4.9%	[33]
Methanol	Toluene	293.2	21.42	27.59	28.8%	20.98	-2.1%	[33]
Methanol	Toluene	293.2	20.50	27.59	34.6%	20.98	2.3%	[30]
Methanol	Toluene	293.2	23.10	27.59	19.4%	20.98	-9.2%	[10]
Methanol	Toluene	293.2	25.40	27.59	8.6%	20.98	-17.4%	[24]
Methanol	Toluene	303.2	18.49	20.86	12.8%	18.17	-1.7%	[33]
Methanol	Toluene	303.2	19.00	20.86	9.8%	18.17	-4.4%	[30]
Methanol	Toluene	303.2	21.20	20.86	-1.6%	18.17	-14.3%	[24]
Methanol	Toluene	313.2	17.35	16.25	-6.3%	15.84	-8.7%	[33]
Methanol	Toluene	313.2	17.60	16.25	-7.7%	15.84	-10.0%	[30]
Methanol	Toluene	313.2	17.40	16.25	-6.6%	15.84	-9.0%	[24]
Methanol	Toluene	323.2	15.10	12.98	-14.0%	13.88	-8.1%	[24]
Methanol	Toluene	381.0	5.00	5.11	2.2%	7.20	44.0%	[12]
Methanol	Toluene	382.2	5.83	5.03	-13.7%	7.11	22.0%	[82]
Methanol	Tributyl Phosphate	298.6	0.46	0.90	95.7%	M.G.	N.A.	[27]
Methanol	Tributyl Phosphate	302.9	0.47	0.88	87.2%	M.G.	N.A.	[27]
Methanol	Tributyl Phosphate	308.6	0.48	0.86	79.2%	M.G.	N.A.	[27]
Methanol	Tributyl Phosphate	313.1	0.48	0.85	77.1%	M.G.	N.A.	[27]
Methanol	Tributyl Phosphate	323.7	0.46	0.81	76.1%	M.G.	N.A.	[27]
Methanol	Tributyl Phosphate	330.0	0.44	0.79	79.5%	M.G.	N.A.	[27]
Methyl Acetate	1-Octanol	298.2	2.69	3.04	13.0%	2.17	-19.3%	[3]
Methyl Acetate	Chloroform	313.4	0.43	0.43	0.0%	0.35	-18.6%	[60]
Methyl Acetate	Chloroform	323.3	0.49	0.46	-6.1%	0.38	-22.4%	[60]
Methyl Acetate	Ethylene Glycol Ethyl Ether	313.2	1.74	1.44	-17.4%	1.35	-22.6%	391
Methyl Acetate	N,N-Dibutylformamide	302.8	1.31	1.20	-8.4%	1.75	33.6%	[13]
Methyl Acetate	N,N-Dibutylformamide	318.3	1.27	1.17	-8.0%	1.68	32.1%	[13]
Methyl Acetate	N,N-Dibutylformamide	332.4	1.23	1.14	-7.6%	1.63	32.1%	[13]
Methyl Acetate	N,N-Dimethylacetamide	303.3	1.47	1.24	-15.9%	1.89	28.2%	[13]
Methyl Acetate	N,N-Dimethylacetamide	317.6	1.23	1.22	-0.7%	1.83	48.9%	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Acetate	N,N-Dimethylacetamide	333.6	1.02	1.21	18.6%	1.71	67.6%	[13]
Methyl Acetate	N-Formylmorpholine	303.5	1.85	1.83	-1.1%	M.G.	N.A.	[43]
Methyl Acetate	N-Formylmorpholine	323.2	1.76	1.74	-1.1%	M.G.	N.A.	[43]
Methyl Acetate	N-Formylmorpholine	342.8	1.69	1.67	-1.2%	M.G.	N.A.	[43]
Methyl Acetate	N-Hexadecane	298.2	3.36	5.00	48.7%	3.15	-6.3%	[6]
Methyl Acetate	N-Methyl-2-Pyrrolidone	323.4	1.62	1.68	3.7%	M.P.	N.A.	[43]
Methyl Acetate	N-Methyl-2-Pyrrolidone	333.2	1.59	1.66	4.4%	M.P.	N.A.	[43]
Methyl Acetate	N-Methyl-2-Pyrrolidone	343.4	1.59	1.63	2.5%	M.P.	N.A.	[43]
Methyl Acetate	N-Methylacetamide	318.4	2.46	2.58	4.7%	2.77	12.4%	[13]
Methyl Acetate	N-Methylacetamide	331.9	2.44	2.50	2.6%	2.70	10.8%	[13]
Methyl Acetate	Sulfolane	303.8	1.95	1.92	-1.3%	M.G.	N.A.	[13]
Methyl Acetate	Sulfolane	317.9	1.91	1.84	-3.8%	M.G.	N.A.	[13]
Methyl Acetate	Sulfolane	333.7	1.88	1.76	-6.3%	M.G.	N.A.	[13]
Methyl Acetate	Tetraethylene Glycol DME	303.2	0.77	0.94	22.7%	0.74	-3.4%	[7]
Methyl Acetate	Tetraethylene Glycol DME	323.2	0.76	0.92	21.5%	0.76	0.4%	[7]
Methyl Acetate	Tributyl Phosphate	298.6	0.95	0.77	-18.9%	M.G.	N.A.	[27]
Methyl Acetate	Tributyl Phosphate	302.9	0.95	0.77	-18.9%	M.G.	N.A.	[27]
Methyl Acetate	Tributyl Phosphate	308.6	0.96	0.76	-20.8%	M.G.	N.A.	[27]
Methyl Acetate	Tributyl Phosphate	313.1	0.96	0.76	-20.8%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	1,1-Dichloroethane	298.2	0.60	0.57	-5.0%	0.57	-5.0%	[16]
Methyl Ethyl Ketone	1,2-Dichloroethane	318.5	0.73	0.71	-2.7%	0.38	-47.9%	[12]
Methyl Ethyl Ketone	1,2-Dichloroethane	333.2	0.75	0.73	-2.6%	0.41	-45.3%	122
Methyl Ethyl Ketone	1,2-Dichloroethane	354.7	0.78	0.77	-1.3%	0.44	-43.6%	[12]
Methyl Ethyl Ketone	1,4-Dioxane	298.2	1.25	1.20	-4.0%	1.25	0.0%	[16]
Methyl Ethyl Ketone	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.07	1.17	9.3%	M.G.	N.A.	[29]
Methyl Ethyl Ketone	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.12	1.16	3.6%	M.G.	N.A.	[29]
Methyl Ethyl Ketone	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.16	1.15	-0.9%	M.G.	N.A.	[29]
Methyl Ethyl Ketone	1-Butanol	278.2	2.74	2.35	-14.1%	2.75	0.5%	79
Methyl Ethyl Ketone	1-Butanol	288.2	2.52	2.26	-10.4%	2.52	-0.1%	79
Methyl Ethyl Ketone	1-Butanol	293.2	2.42	2.22	-8.2%	2.42	0.1%	79
Methyl Ethyl Ketone	1-Butanol	298.2	2.35	2.18	-7.1%	2.32	-1.1%	79
Methyl Ethyl Ketone	1-Butanol	298.2	2.06	2.18	5.8%	2.32	12.6%	[16]
Methyl Ethyl Ketone	1-Butanol	303.2	2.21	2.15	-2.8%	2.24	1.3%	79
Methyl Ethyl Ketone	1-Butanol	308.2	2.09	2.11	1.1%	2.15	3.0%	79
Methyl Ethyl Ketone	1-Butanol	308.2	2.15	2.11	-1.9%	2.15	0.0%	[30]
Methyl Ethyl Ketone	1-Butanol	313.2	2.03	2.08	2.5%	2.07	2.1%	79
Methyl Ethyl Ketone	1-Butanol	318.2	1.95	2.05	5.1%	2.00	2.6%	[30]
Methyl Ethyl Ketone	1-Butanol	323.2	1.92	2.02	5.1%	1.94	0.9%	79
Methyl Ethyl Ketone	1-Butanol	328.2	1.74	1.99	14.4%	1.87	7.5%	[30]
Methyl Ethyl Ketone	1-Ethylpyrrolidin-2-One	298.2	1.21	1.20	-0.8%	M.P.	N.A.	[29]
Methyl Ethyl Ketone	1-Ethylpyrrolidin-2-One	308.2	1.19	1.19	0.0%	M.P.	N.A.	[29]
Methyl Ethyl Ketone	1-Ethylpyrrolidin-2-One	318.2	1.16	1.18	1.7%	M.P.	N.A.	[29]
Methyl Ethyl Ketone	1-Octanol	293.2	2.43	2.29	-5.9%	2.20	-9.6%	76
Methyl Ethyl Ketone	1-Octanol	293.2	2.02	2.29	13.4%	2.20	8.9%	[10]
Methyl Ethyl Ketone	1-Octanol	298.2	2.24	2.23	-0.6%	2.10	-6.4%	76
Methyl Ethyl Ketone	1-Octanol	298.2	2.22	2.23	0.5%	2.10	-5.4%	[3]
Methyl Ethyl Ketone	1-Octanol	298.2	2.09	2.23	6.7%	2.10	0.5%	[16]
Methyl Ethyl Ketone	1-Octanol	303.2	2.21	2.18	-1.5%	2.00	-9.6%	76
Methyl Ethyl Ketone	1-Octanol	308.2	2.02	2.12	5.0%	1.92	-4.9%	76
Methyl Ethyl Ketone	1-Octanol	313.2	1.95	2.08	6.5%	1.84	-5.8%	76

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Ethyl Ketone	1-Octanol	323.2	1.79	1.99	11.1%	1.70	-5.1%	76
Methyl Ethyl Ketone	1-Pentanol	303.5	2.12	2.13	0.5%	2.16	1.9%	[33]
Methyl Ethyl Ketone	1-Pentanol	308.2	2.19	2.09	-4.6%	2.08	-5.0%	[30]
Methyl Ethyl Ketone	1-Pentanol	313.2	2.01	2.05	2.0%	2.00	-0.5%	[33]
Methyl Ethyl Ketone	1-Pentanol	318.2	2.16	2.02	-6.5%	1.93	-10.6%	[30]
Methyl Ethyl Ketone	1-Pentanol	323.5	1.85	1.98	7.0%	1.85	0.0%	[33]
Methyl Ethyl Ketone	1-Pentanol	328.2	1.84	1.95	6.0%	1.80	-2.2%	[30]
Methyl Ethyl Ketone	1-Propanol	298.2	2.28	2.27	-0.4%	2.42	6.1%	[16]
Methyl Ethyl Ketone	2,2,4-Trimethylpentane	293.2	5.16	4.64	-10.1%	5.14	-0.5%	58
Methyl Ethyl Ketone	2,2,4-Trimethylpentane	293.2	3.86	4.64	20.2%	5.14	33.2%	[10]
Methyl Ethyl Ketone	2,2,4-Trimethylpentane	298.2	4.18	4.41	5.5%	4.90	17.2%	[16]
Methyl Ethyl Ketone	2,2,4-Trimethylpentane	313.2	3.75	3.85	2.7%	4.30	14.7%	58
Methyl Ethyl Ketone	2,6-Dimethylpyridine	298.2	1.02	1.29	26.5%	1.66	62.7%	[16]
Methyl Ethyl Ketone	2-Butanol	278.2	2.85	2.45	-14.1%	2.75	-3.5%	68
Methyl Ethyl Ketone	2-Butanol	288.2	2.37	2.34	-1.4%	2.52	6.2%	68
Methyl Ethyl Ketone	2-Butanol	293.2	2.30	2.29	-0.6%	2.42	5.1%	68
Methyl Ethyl Ketone	2-Butanol	298.2	2.16	2.25	4.3%	2.32	7.6%	68
Methyl Ethyl Ketone	2-Butanol	303.2	2.12	2.21	4.4%	2.24	5.9%	68
Methyl Ethyl Ketone	2-Butanol	308.2	1.96	2.16	10.5%	2.15	10.0%	68
Methyl Ethyl Ketone	2-Butanol	313.2	1.84	2.13	15.8%	2.07	12.5%	68
Methyl Ethyl Ketone	2-Butanol	323.2	1.75	2.05	17.4%	1.94	11.1%	68
Methyl Ethyl Ketone	2-Methyl-1-Propanol	278.2	2.64	2.29	-13.1%	2.75	4.3%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	288.2	2.40	2.20	-8.5%	2.52	4.8%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	293.2	2.27	2.16	-5.0%	2.42	6.5%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	298.2	2.21	2.13	-3.8%	2.32	4.8%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	303.2	2.10	2.09	-0.5%	2.24	6.6%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	308.2	1.96	2.06	5.2%	2.15	9.8%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	313.2	1.89	2.02	6.9%	2.07	9.5%	78
Methyl Ethyl Ketone	2-Methyl-1-Propanol	323.2	1.74	1.96	12.7%	1.94	11.5%	78
Methyl Ethyl Ketone	2-Methyl-2-Propanol	298.2	1.66	1.93	16.3%	2.38	43.4%	[16]
Methyl Ethyl Ketone	2-Methyl-2-Propanol	303.2	1.73	1.90	9.9%	2.29	32.4%	77
Methyl Ethyl Ketone	2-Methyl-2-Propanol	308.2	1.71	1.88	9.8%	2.20	28.5%	77
Methyl Ethyl Ketone	2-Methyl-2-Propanol	313.2	1.67	1.85	10.8%	2.12	27.0%	77
Methyl Ethyl Ketone	2-Methyl-2-Propanol	318.2	1.61	1.83	13.7%	2.05	27.3%	77
Methyl Ethyl Ketone	2-Methyl-2-Propanol	323.2	1.58	1.80	14.2%	1.98	25.6%	77
Methyl Ethyl Ketone	2-Pyrrolidone	303.2	2.81	2.46	-12.3%	M.G.	N.A.	[35]
Methyl Ethyl Ketone	2-Pyrrolidone	313.2	2.76	2.37	-14.0%	M.G.	N.A.	[35]
Methyl Ethyl Ketone	2-Pyrrolidone	323.2	2.71	2.28	-15.9%	M.G.	N.A.	[35]
Methyl Ethyl Ketone	2-Pyrrolidone	333.2	2.67	2.21	-17.2%	M.G.	N.A.	[35]
Methyl Ethyl Ketone	Acetic Acid	298.2	0.93	0.69	-25.8%	1.22	31.2%	[16]
Methyl Ethyl Ketone	Acetone	298.2	1.06	1.08	1.9%	1.02	-3.8%	[16]
Methyl Ethyl Ketone	Acetone	298.3	1.06	1.08	1.9%	1.02	-3.8%	[17]
Methyl Ethyl Ketone	Acetone	308.2	1.10	1.08	-1.8%	1.01	-8.2%	[17]
Methyl Ethyl Ketone	Acetone	318.4	1.05	1.07	1.9%	1.01	-3.8%	[17]
Methyl Ethyl Ketone	Acetone	328.4	1.10	1.07	-2.7%	1.01	-8.2%	[17]
Methyl Ethyl Ketone	Acetonitrile	298.2	1.22	1.30	6.6%	1.22	0.0%	[16]
Methyl Ethyl Ketone	Acetonitrile	333.7	1.26	1.22	-3.4%	1.18	-6.6%	205
Methyl Ethyl Ketone	Acetophenone	298.2	1.00	0.95	-5.0%	1.16	16.0%	[16]
Methyl Ethyl Ketone	Aniline	298.2	0.61	0.95	55.7%	0.75	23.0%	[16]
Methyl Ethyl Ketone	Anisole	298.2	0.95	1.00	5.3%	1.06	11.6%	[16]
Methyl Ethyl Ketone	Anisole	333.2	1.05	1.02	-2.8%	1.09	3.9%	51
Methyl Ethyl Ketone	Anisole	353.2	1.09	1.02	-6.6%	1.10	0.7%	51

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Ethyl Ketone	Benzene	298.2	1.22	1.19	-2.5%	1.25	2.5%	[16]
Methyl Ethyl Ketone	Benzene	353.3	1.38	1.18	-14.5%	1.26	-8.7%	[11]
Methyl Ethyl Ketone	Benzonitrile	298.2	0.88	1.05	19.3%	M.G.	N.A.	[16]
Methyl Ethyl Ketone	Benzyl Alcohol	298.2	0.78	0.73	-6.4%	1.31	67.9%	[16]
Methyl Ethyl Ketone	Bromobenzene	298.2	1.18	1.40	18.6%	0.93	-21.2%	[16]
Methyl Ethyl Ketone	Bromoethane	298.2	1.03	1.12	8.7%	1.12	8.7%	[16]
Methyl Ethyl Ketone	Butyl Ether	298.2	2.26	2.09	-7.5%	2.26	0.0%	[16]
Methyl Ethyl Ketone	Butyronitrile	298.2	0.94	1.05	11.7%	1.05	11.7%	[16]
Methyl Ethyl Ketone	Carbon Disulfide	298.2	5.14	5.73	11.5%	5.43	5.6%	[16]
Methyl Ethyl Ketone	Carbon Disulfide	298.3	4.92	5.73	16.5%	5.42	10.2%	[17]
Methyl Ethyl Ketone	Carbon Disulfide	308.4	4.80	5.30	10.4%	5.13	6.9%	[17]
Methyl Ethyl Ketone	Carbon Disulfide	318.7	4.44	4.92	10.8%	4.87	9.7%	[17]
Methyl Ethyl Ketone	Carbon Tetrachloride	314.9	2.10	1.69	-19.5%	2.34	11.4%	[12]
Methyl Ethyl Ketone	Carbon Tetrachloride	328.3	2.06	1.65	-19.9%	2.26	9.7%	[12]
Methyl Ethyl Ketone	Carbon Tetrachloride	340.2	2.02	1.62	-19.8%	2.18	7.9%	[12]
Methyl Ethyl Ketone	Carbon Tetrachloride	346.3	1.98	1.60	-19.2%	2.14	8.1%	[12]
Methyl Ethyl Ketone	Chlorobenzene	298.2	1.03	1.34	30.1%	1.27	23.3%	[16]
Methyl Ethyl Ketone	Chloroform	318.2	0.26	0.26	-1.7%	0.35	32.3%	232
Methyl Ethyl Ketone	Chloroform	328.2	0.31	0.29	-7.5%	0.39	24.4%	232
Methyl Ethyl Ketone	Cyclohexane	298.2	5.27	5.56	5.5%	5.29	0.4%	[16]
Methyl Ethyl Ketone	Cyclohexane	323.2	4.33	4.44	2.6%	4.23	-2.2%	335
Methyl Ethyl Ketone	Cyclohexane	350.8	3.70	3.64	-1.6%	3.44	-7.0%	[12]
Methyl Ethyl Ketone	Cyclohexanone	298.2	1.00	1.04	4.0%	1.07	7.0%	[16]
Methyl Ethyl Ketone	Dichloromethane	298.2	0.44	0.40	-9.1%	0.44	0.0%	[16]
Methyl Ethyl Ketone	Diethyl Ether	298.2	1.85	1.68	-9.2%	2.03	9.7%	[16]
Methyl Ethyl Ketone	Diethyl Phthalate	303.2	0.92	0.87	-4.9%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Diethyl Phthalate	313.2	0.92	0.87	-4.9%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Diethyl Phthalate	323.2	0.93	0.87	-6.1%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Diethyl Phthalate	333.2	0.93	0.87	-6.7%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Diisopropyl Ether	298.2	2.07	2.07	0.0%	2.65	28.0%	[16]
Methyl Ethyl Ketone	Dimethyl Sulfoxide	298.2	2.05	2.23	8.8%	2.40	17.1%	[16]
Methyl Ethyl Ketone	Epsilon-Caprolactone	303.2	1.37	1.32	-3.6%	M.G.	N.A.	[41]
Methyl Ethyl Ketone	Epsilon-Caprolactone	318.2	1.35	1.29	-4.4%	M.G.	N.A.	[41]
Methyl Ethyl Ketone	Epsilon-Caprolactone	333.2	1.34	1.27	-5.2%	M.G.	N.A.	[41]
Methyl Ethyl Ketone	Ethanol	278.2	2.81	2.39	-15.0%	2.95	4.9%	264
Methyl Ethyl Ketone	Ethanol	288.2	2.60	2.34	-9.8%	2.76	6.3%	264
Methyl Ethyl Ketone	Ethanol	298.2	2.49	2.29	-8.1%	2.59	3.9%	264
Methyl Ethyl Ketone	Ethanol	298.2	2.45	2.29	-6.5%	2.59	5.7%	[16]
Methyl Ethyl Ketone	Ethanol	303.2	2.57	2.26	-12.1%	2.51	-2.3%	[18]
Methyl Ethyl Ketone	Ethanol	308.2	2.38	2.24	-5.8%	2.43	2.2%	264
Methyl Ethyl Ketone	Ethanol	313.2	2.32	2.21	-4.6%	2.36	1.8%	264
Methyl Ethyl Ketone	Ethanol	313.2	2.31	2.21	-4.3%	2.36	2.2%	[18]
Methyl Ethyl Ketone	Ethanol	313.9	2.28	2.21	-3.1%	2.35	3.1%	[18]
Methyl Ethyl Ketone	Ethanol	323.2	2.25	2.16	-4.1%	2.23	-1.0%	264
Methyl Ethyl Ketone	Ethanol	323.2	2.22	2.16	-2.7%	2.23	0.5%	[18]
Methyl Ethyl Ketone	Ethanol	351.5	1.97	2.01	2.0%	1.90	-3.6%	[11]
Methyl Ethyl Ketone	Ethyl Acetate	313.0	1.11	1.02	-8.1%	1.11	0.0%	[12]
Methyl Ethyl Ketone	Ethyl Acetate	328.4	1.10	1.02	-7.3%	1.11	0.9%	[17]
Methyl Ethyl Ketone	Ethyl Acetate	333.5	1.08	1.02	-5.6%	1.11	2.8%	[12]
Methyl Ethyl Ketone	Ethyl Acetate	348.3	1.04	1.02	-1.9%	1.11	6.7%	[12]
Methyl Ethyl Ketone	Glutaronitrile	303.2	1.74	1.70	-2.3%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Glutaronitrile	313.2	1.74	1.65	-5.2%	M.G.	N.A.	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Ethyl Ketone	Glutaronitrile	323.2	1.73	1.61	-6.9%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Glutaronitrile	333.2	1.73	1.57	-9.2%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	Isopropanol	278.2	3.01	2.48	-17.6%	2.71	-9.9%	262
Methyl Ethyl Ketone	Isopropanol	288.2	2.72	2.40	-11.8%	2.50	-8.1%	262
Methyl Ethyl Ketone	Isopropanol	293.2	2.60	2.36	-9.2%	2.41	-7.3%	262
Methyl Ethyl Ketone	Isopropanol	298.2	2.50	2.32	-7.1%	2.32	-7.1%	262
Methyl Ethyl Ketone	Isopropanol	298.2	2.43	2.32	-4.5%	2.32	-4.5%	[16]
Methyl Ethyl Ketone	Isopropanol	308.2	2.35	2.25	-4.4%	2.16	-8.2%	262
Methyl Ethyl Ketone	Isopropanol	313.2	2.20	2.22	0.7%	2.09	-5.2%	262
Methyl Ethyl Ketone	Isopropanol	323.2	2.06	2.15	4.3%	1.96	-5.0%	262
Methyl Ethyl Ketone	M-Cresol	298.2	0.08	0.08	0.0%	0.08	0.0%	[16]
Methyl Ethyl Ketone	Methanol	288.2	2.55	2.16	-15.1%	2.35	-7.7%	263
Methyl Ethyl Ketone	Methanol	298.2	2.51	2.13	-15.1%	2.28	-9.1%	263
Methyl Ethyl Ketone	Methanol	298.2	2.49	2.13	-14.5%	2.28	-8.4%	[16]
Methyl Ethyl Ketone	Methanol	303.2	2.50	2.11	-15.6%	2.25	-10.0%	263
Methyl Ethyl Ketone	Methanol	303.2	2.32	2.11	-9.1%	2.25	-3.0%	[18]
Methyl Ethyl Ketone	Methanol	308.2	2.46	2.09	-15.0%	2.22	-9.7%	263
Methyl Ethyl Ketone	Methanol	308.2	2.26	2.09	-7.5%	2.22	-1.8%	[18]
Methyl Ethyl Ketone	Methanol	308.7	2.27	2.09	-7.9%	2.21	-2.6%	[17]
Methyl Ethyl Ketone	Methanol	313.2	2.43	2.07	-14.8%	2.19	-9.9%	263
Methyl Ethyl Ketone	Methanol	313.2	2.22	2.07	-6.8%	2.19	-1.4%	[18]
Methyl Ethyl Ketone	Methanol	318.3	2.20	2.05	-6.8%	2.16	-1.8%	[18]
Methyl Ethyl Ketone	Methanol	318.5	2.21	2.05	-7.2%	2.15	-2.7%	[17]
Methyl Ethyl Ketone	Methanol	323.2	2.29	2.03	-11.3%	2.13	-6.9%	263
Methyl Ethyl Ketone	Methanol	328.5	2.11	2.00	-5.2%	2.10	-0.5%	[17]
Methyl Ethyl Ketone	Methanol	337.0	2.07	1.96	-5.3%	2.05	-1.0%	[17]
Methyl Ethyl Ketone	Methyl Isobutyl Ketone	328.2	1.13	1.07	-5.3%	1.02	-9.7%	[49]
Methyl Ethyl Ketone	Methyl Isobutyl Ketone	348.2	1.09	1.06	-2.8%	1.02	-6.4%	[49]
Methyl Ethyl Ketone	Methyl Isobutyl Ketone	388.2	1.06	1.04	-1.9%	1.01	-4.7%	[49]
Methyl Ethyl Ketone	N,N-Dibutylformamide	302.8	0.95	1.01	6.1%	1.12	17.6%	[13]
Methyl Ethyl Ketone	N,N-Dibutylformamide	318.3	0.96	0.99	2.9%	1.12	16.4%	[13]
Methyl Ethyl Ketone	N,N-Dibutylformamide	332.4	0.97	0.98	1.1%	1.12	15.6%	[13]
Methyl Ethyl Ketone	N,N-Diethylacetamide	303.2	1.01	1.05	4.0%	0.88	-12.9%	[39]
Methyl Ethyl Ketone	N,N-Diethylacetamide	313.2	1.02	1.04	2.0%	0.89	-12.7%	[39]
Methyl Ethyl Ketone	N,N-Diethylacetamide	323.2	1.03	1.04	1.0%	0.90	-12.6%	[39]
Methyl Ethyl Ketone	N,N-Diethylacetamide	333.2	1.04	1.04	0.0%	0.91	-12.5%	[39]
Methyl Ethyl Ketone	N,N-Dimethylacetamide	333.6	1.38	1.17	-15.3%	0.81	-41.4%	[13]
Methyl Ethyl Ketone	N,N-Dimethylformamide	298.2	1.15	1.52	32.2%	1.15	0.0%	[16]
Methyl Ethyl Ketone	N-Decane	298.2	4.13	4.21	1.9%	4.47	8.2%	[16]
Methyl Ethyl Ketone	N-Ethylacetamide	303.2	2.08	2.02	-2.9%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	N-Ethylacetamide	313.2	2.02	1.99	-1.5%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	N-Ethylacetamide	323.2	1.99	1.96	-1.5%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	N-Ethylacetamide	333.2	1.94	1.92	-1.0%	M.G.	N.A.	[39]
Methyl Ethyl Ketone	N-Formylmorpholine	303.5	1.93	1.84	-4.7%	M.G.	N.A.	[43]
Methyl Ethyl Ketone	N-Formylmorpholine	323.2	1.84	1.75	-4.9%	M.G.	N.A.	[43]
Methyl Ethyl Ketone	N-Formylmorpholine	342.8	1.75	1.67	-4.6%	M.G.	N.A.	[43]
Methyl Ethyl Ketone	N-Heptane	298.2	4.26	4.54	6.6%	5.18	21.6%	[16]
Methyl Ethyl Ketone	N-Heptane	312.9	4.23	3.98	-5.9%	4.56	7.8%	[18]
Methyl Ethyl Ketone	N-Heptane	313.2	4.12	3.97	-3.6%	4.55	10.4%	[18]
Methyl Ethyl Ketone	N-Heptane	323.2	3.69	3.66	-0.8%	4.19	13.6%	[18]
Methyl Ethyl Ketone	N-Heptane	333.0	3.27	3.41	4.3%	3.89	19.0%	[18]
Methyl Ethyl Ketone	N-Heptane	343.2	3.12	3.18	1.9%	3.62	16.0%	[18]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Ethyl Ketone	N-Hexadecane	298.2	3.92	3.62	-7.7%	3.62	-7.7%	[6]
Methyl Ethyl Ketone	N-Hexadecane	298.2	3.25	3.62	11.4%	3.62	11.4%	[16]
Methyl Ethyl Ketone	N-Hexadecane	333.2	2.70	2.68	-0.8%	2.71	0.4%	83
Methyl Ethyl Ketone	N-Hexadecane	353.2	2.26	2.34	3.5%	2.36	4.3%	83
Methyl Ethyl Ketone	N-Hexane	298.0	4.38	4.66	6.4%	5.55	26.7%	[12]
Methyl Ethyl Ketone	N-Hexane	298.2	4.53	4.65	2.6%	5.54	22.3%	[16]
Methyl Ethyl Ketone	N-Hexane	303.4	4.31	4.43	2.8%	5.28	22.5%	[18]
Methyl Ethyl Ketone	N-Hexane	313.2	3.98	4.07	2.3%	4.86	22.1%	[18]
Methyl Ethyl Ketone	N-Hexane	313.3	3.92	4.06	3.6%	4.85	23.7%	[18]
Methyl Ethyl Ketone	N-Hexane	315.3	3.97	4.00	0.8%	4.77	20.2%	[12]
Methyl Ethyl Ketone	N-Hexane	323.2	3.69	3.75	1.6%	4.48	21.4%	[18]
Methyl Ethyl Ketone	N-Hexane	332.0	3.60	3.52	-2.2%	4.19	16.4%	[12]
Methyl Ethyl Ketone	N-Hexane	340.3	3.40	3.32	-2.4%	3.94	15.9%	[12]
Methyl Ethyl Ketone	Nitrobenzene	298.2	1.04	0.95	-8.7%	1.26	21.2%	[16]
Methyl Ethyl Ketone	Nitromethane	298.2	1.22	1.13	-7.4%	1.18	-3.3%	[16]
Methyl Ethyl Ketone	N-Methyl-2-Pyrrolidone	323.4	1.45	1.49	2.8%	M.P.	N.A.	[43]
Methyl Ethyl Ketone	N-Methyl-2-Pyrrolidone	333.2	1.45	1.47	1.4%	M.P.	N.A.	[43]
Methyl Ethyl Ketone	N-Methyl-2-Pyrrolidone	343.4	1.42	1.45	2.1%	M.P.	N.A.	[43]
Methyl Ethyl Ketone	N-Methylacetamide	303.1	2.24	2.26	1.0%	2.33	4.2%	[13]
Methyl Ethyl Ketone	N-Methylacetamide	318.4	2.18	2.21	1.4%	2.23	2.3%	[13]
Methyl Ethyl Ketone	N-Methylacetamide	333.2	2.11	2.15	2.1%	2.14	1.6%	[13]
Methyl Ethyl Ketone	N-Methylformamide	303.2	2.56	2.52	-1.6%	M.P.	N.A.	[35]
Methyl Ethyl Ketone	N-Methylformamide	313.2	2.54	2.46	-3.0%	M.P.	N.A.	[35]
Methyl Ethyl Ketone	N-Methylformamide	323.2	2.51	2.39	-4.8%	M.P.	N.A.	[35]
Methyl Ethyl Ketone	N-Methylformamide	333.2	2.49	2.33	-6.4%	M.P.	N.A.	[35]
Methyl Ethyl Ketone	N-Octane	293.2	4.15	4.66	12.3%	5.14	23.9%	[10]
Methyl Ethyl Ketone	N-Pentane	298.2	5.47	4.78	-12.6%	6.02	10.1%	[16]
Methyl Ethyl Ketone	N-Pentane	303.2	5.19	4.56	-12.1%	5.76	11.0%	[18]
Methyl Ethyl Ketone	P-Xylene	298.2	1.42	1.48	4.2%	1.80	26.8%	[16]
Methyl Ethyl Ketone	Pyridine	298.2	0.97	1.30	34.0%	1.10	13.4%	[16]
Methyl Ethyl Ketone	Sulfolane	303.1	1.99	1.97	-1.2%	M.G.	N.A.	[13]
Methyl Ethyl Ketone	Sulfolane	317.9	1.95	1.87	-4.1%	M.G.	N.A.	[13]
Methyl Ethyl Ketone	Sulfolane	332.6	1.91	1.79	-6.3%	M.G.	N.A.	[13]
Methyl Ethyl Ketone	Tetraethylene Glycol DME	304.6	0.86	0.85	-1.0%	0.75	-12.7%	[7]
Methyl Ethyl Ketone	Tetraethylene Glycol DME	323.2	0.85	0.84	-0.7%	0.83	-1.9%	[7]
Methyl Ethyl Ketone	Tetraethylene Glycol DME	343.2	0.84	0.84	0.5%	0.98	17.2%	[7]
Methyl Ethyl Ketone	Toluene	298.2	1.37	1.34	-2.2%	1.48	8.0%	[16]
Methyl Ethyl Ketone	Toluene	323.2	1.47	1.31	-10.8%	1.50	2.1%	267
Methyl Ethyl Ketone	Toluene	342.7	1.39	1.29	-7.2%	1.49	7.2%	[12]
Methyl Ethyl Ketone	Toluene	362.7	1.35	1.27	-5.9%	1.45	7.4%	[12]
Methyl Ethyl Ketone	Toluene	381.0	1.33	1.25	-6.0%	1.39	4.5%	[12]
Methyl Ethyl Ketone	Tributyl Phosphate	298.6	0.79	0.69	-12.7%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	Tributyl Phosphate	302.9	0.80	0.69	-13.8%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	Tributyl Phosphate	308.6	0.81	0.69	-14.8%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	Tributyl Phosphate	313.1	0.83	0.68	-18.1%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	Tributyl Phosphate	323.7	0.80	0.68	-15.0%	M.G.	N.A.	[27]
Methyl Ethyl Ketone	Triethylamine	298.2	2.91	2.92	0.3%	2.60	-10.7%	[16]
Methyl Formate	1-Octanol	298.2	3.58	3.49	-2.5%	2.94	-17.9%	[3]
Methyl Formate	Ethylene Glycol Ethyl Ether	308.2	1.75	1.63	-7.1%	M.P.	N.A.	391
Methyl Formate	N,N-Dibutylformamide	302.8	1.17	1.11	-4.7%	1.25	7.3%	[13]
Methyl Formate	N,N-Dibutylformamide	318.3	1.20	1.08	-10.3%	1.26	4.7%	[13]
Methyl Formate	N,N-Dibutylformamide	332.4	1.24	1.05	-15.1%	1.27	2.7%	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Formate	N,N-Dimethylacetamide	303.3	1.11	1.13	1.5%	M.P.	N.A.	[13]
Methyl Formate	N,N-Dimethylacetamide	317.6	1.19	1.12	-6.0%	M.P.	N.A.	[13]
Methyl Formate	N,N-Dimethylacetamide	333.0	1.27	1.11	-12.9%	M.P.	N.A.	[13]
Methyl Formate	N-Hexadecane	298.2	4.23	4.15	-1.9%	3.75	-11.3%	[6]
Methyl Formate	N-Methylacetamide	318.4	2.13	2.03	-4.6%	M.P.	N.A.	[13]
Methyl Formate	N-Methylacetamide	331.9	2.19	1.98	-9.6%	M.P.	N.A.	[13]
Methyl Formate	Sulfolane	303.8	1.43	1.34	-6.6%	M.G.	N.A.	[13]
Methyl Formate	Sulfolane	317.9	1.42	1.31	-7.8%	M.G.	N.A.	[13]
Methyl Formate	Sulfolane	333.7	1.41	1.28	-9.1%	M.G.	N.A.	[13]
Methyl Formate	Tetraethylene Glycol DME	303.2	0.60	0.83	37.6%	M.P.	N.A.	[7]
Methyl Formate	Tetraethylene Glycol DME	323.2	0.64	0.82	27.9%	M.P.	N.A.	[7]
Methyl Formate	Tetraethylene Glycol DME	343.2	0.72	0.81	12.3%	M.P.	N.A.	[7]
Methyl Iodide	1,2-Dichloroethane	293.2	1.34	1.28	-4.5%	0.85	-36.6%	[10]
Methyl Iodide	1-Butanol	293.2	3.05	3.10	1.6%	3.23	5.9%	[10]
Methyl Iodide	1-Chlorobutane	293.2	1.31	1.29	-1.5%	M.P.	N.A.	[10]
Methyl Iodide	1-Octanol	293.2	2.06	1.92	-6.8%	2.08	1.0%	[10]
Methyl Iodide	2,2,4-Trimethylpentane	293.2	1.95	2.31	18.5%	1.88	-3.6%	[10]
Methyl Iodide	2-Nitropropane	293.2	2.03	1.98	-2.5%	1.95	-3.9%	[10]
Methyl Iodide	Acetonitrile	293.2	3.86	4.62	19.7%	M.P.	N.A.	[10]
Methyl Iodide	Acetophenone	293.2	1.23	1.26	2.4%	1.25	1.6%	[10]
Methyl Iodide	Aniline	293.2	2.83	2.07	-26.9%	M.P.	N.A.	[10]
Methyl Iodide	Anisole	293.2	1.14	1.07	-6.1%	0.93	-18.4%	[10]
Methyl Iodide	Benzene	293.2	1.18	1.09	-7.6%	1.12	-5.1%	[58]
Methyl Iodide	Benzene	293.2	1.15	1.09	-5.2%	1.12	-2.6%	[10]
Methyl Iodide	Benzonitrile	293.2	1.58	1.43	-9.5%	M.G.	N.A.	[10]
Methyl Iodide	Benzonitrile	293.2	1.41	1.43	1.4%	M.G.	N.A.	[10]
Methyl Iodide	Benzyl Acetate	298.2	1.13	1.04	-8.0%	1.00	-11.5%	[10]
Methyl Iodide	Carbon Tetrachloride	293.2	1.37	1.28	-6.6%	1.33	-2.9%	[10]
Methyl Iodide	Cyclohexanone	293.2	1.05	1.06	1.0%	M.P.	N.A.	[10]
Methyl Iodide	Ethanol	293.2	5.26	5.47	4.0%	5.05	-4.0%	[10]
Methyl Iodide	Ethyl Acetate	293.2	1.34	1.44	7.5%	1.36	1.5%	[10]
Methyl Iodide	Methyl Ethyl Ketone	293.2	1.45	1.42	-2.1%	1.47	1.4%	[10]
Methyl Iodide	N,N-Dimethylformamide	293.2	1.65	1.83	10.9%	M.P.	N.A.	[10]
Methyl Iodide	N-Heptane	293.2	1.94	1.90	-2.1%	2.01	3.6%	[10]
Methyl Iodide	Nitrobenzene	293.2	1.68	1.44	-14.3%	M.P.	N.A.	[10]
Methyl Iodide	Nitromethane	293.2	4.70	5.58	18.7%	4.47	-4.9%	[10]
Methyl Iodide	N-Octane	293.2	1.86	1.73	-7.0%	1.88	1.1%	[10]
Methyl Iodide	Phenol	323.2	2.33	2.39	2.6%	M.P.	N.A.	[10]
Methyl Iodide	Propionitrile	293.2	2.14	2.30	7.5%	M.P.	N.A.	[10]
Methyl Iodide	P-Xylene	293.2	1.06	1.11	4.7%	1.18	11.3%	[10]
Methyl Iodide	Quinoline	298.2	1.25	1.20	-4.0%	M.G.	N.A.	[10]
Methyl Iodide	Toluene	293.2	1.15	1.06	-7.8%	1.15	0.0%	[10]
Methyl Isobutyl Ketone	N,N-Dibutylformamide	302.8	1.08	1.05	-2.7%	1.08	0.1%	[13]
Methyl Isobutyl Ketone	N,N-Dibutylformamide	318.3	1.05	1.04	-0.9%	1.09	3.9%	[13]
Methyl Isobutyl Ketone	N,N-Dibutylformamide	332.5	1.04	1.03	-1.0%	1.11	6.7%	[13]
Methyl Isobutyl Ketone	N,N-Dimethylacetamide	303.2	1.44	1.70	18.1%	0.83	-42.4%	[13]
Methyl Isobutyl Ketone	N,N-Dimethylacetamide	317.6	1.33	1.63	22.7%	0.83	-37.5%	[13]
Methyl Isobutyl Ketone	N,N-Dimethylacetamide	333.2	1.22	1.57	28.4%	0.84	-31.3%	[13]
Methyl Isobutyl Ketone	N-Formylmorpholine	323.2	3.23	3.41	5.6%	M.G.	N.A.	[43]
Methyl Isobutyl Ketone	N-Formylmorpholine	342.8	2.93	3.06	4.4%	M.G.	N.A.	[43]
Methyl Isobutyl Ketone	N-Methylacetamide	303.2	3.48	3.47	-0.2%	2.84	-18.3%	[13]
Methyl Isobutyl Ketone	N-Methylacetamide	318.4	3.40	3.33	-1.9%	2.74	-19.3%	[13]

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Methyl Isobutyl Ketone	N-Methylacetamide	333.3	3.23	3.18	-1.6%	2.65	-18.0%	[13]
Methyl Isobutyl Ketone	Sulfolane	303.8	3.89	4.41	13.3%	M.G.	N.A.	[13]
Methyl Isobutyl Ketone	Sulfolane	317.9	3.77	3.93	4.2%	M.G.	N.A.	[13]
Methyl Isobutyl Ketone	Sulfolane	333.6	3.63	3.51	-3.2%	M.G.	N.A.	[13]
Methyl Isobutyl Ketone	Tributyl Phosphate	298.6	0.36	0.73	102.8%	M.G.	N.A.	[27]
Methyl Isobutyl Ketone	Tributyl Phosphate	302.9	0.38	0.73	92.1%	M.G.	N.A.	[27]
Methyl Isobutyl Ketone	Tributyl Phosphate	308.6	0.38	0.73	92.1%	M.G.	N.A.	[27]
Methyl Isobutyl Ketone	Tributyl Phosphate	313.1	0.39	0.73	87.2%	M.G.	N.A.	[27]
Methyl Tert-Butyl Ether	1,5-Dimethyl-2-Pyrrolidinone	298.2	2.70	2.71	0.4%	M.G.	N.A.	[29]
Methyl Tert-Butyl Ether	1,5-Dimethyl-2-Pyrrolidinone	308.2	2.68	2.59	-3.4%	M.G.	N.A.	[29]
Methyl Tert-Butyl Ether	1,5-Dimethyl-2-Pyrrolidinone	318.2	2.66	2.47	-7.1%	M.G.	N.A.	[29]
Methyl Tert-Butyl Ether	1-Ethylpyrrolidin-2-One	298.2	2.92	2.71	-7.2%	M.P.	N.A.	[29]
Methyl Tert-Butyl Ether	1-Ethylpyrrolidin-2-One	308.2	2.75	2.59	-5.8%	M.P.	N.A.	[29]
Methyl Tert-Butyl Ether	1-Ethylpyrrolidin-2-One	318.2	2.74	2.48	-9.5%	M.P.	N.A.	[29]
Methyl Tert-Butyl Ether	1-Octanol	298.2	1.25	1.24	-0.8%	1.52	21.6%	[3]
Methyl Tert-Butyl Ether	2-Methylpentane	303.2	1.25	1.36	8.8%	1.28	2.4%	[56]
Methyl Tert-Butyl Ether	2-Methylpentane	323.2	1.19	1.32	10.9%	1.24	4.2%	[56]
Methyl Tert-Butyl Ether	2-Pyrrolidone	303.2	8.24	9.59	16.5%	M.G.	N.A.	[35]
Methyl Tert-Butyl Ether	2-Pyrrolidone	313.2	8.04	8.61	7.1%	M.G.	N.A.	[35]
Methyl Tert-Butyl Ether	2-Pyrrolidone	323.2	7.86	7.77	-1.1%	M.G.	N.A.	[35]
Methyl Tert-Butyl Ether	2-Pyrrolidone	333.2	7.66	7.07	-7.6%	M.G.	N.A.	[35]
Methyl Tert-Butyl Ether	Cyclohexane	313.2	1.41	1.46	3.5%	1.27	-9.9%	[56]
Methyl Tert-Butyl Ether	Cyclohexane	333.2	1.32	1.41	6.8%	1.21	-8.3%	[56]
Methyl Tert-Butyl Ether	Cyclopentane	313.2	1.19	1.39	16.8%	1.28	7.6%	[56]
Methyl Tert-Butyl Ether	Cyclopentane	323.2	1.12	1.37	22.3%	1.25	11.6%	[56]
Methyl Tert-Butyl Ether	Diethyl Phthalate	303.2	1.58	1.49	-5.7%	1.06	-32.9%	[39]
Methyl Tert-Butyl Ether	Diethyl Phthalate	313.2	1.57	1.45	-7.6%	1.04	-33.8%	[39]
Methyl Tert-Butyl Ether	Diethyl Phthalate	323.2	1.57	1.42	-9.6%	1.03	-34.4%	[39]
Methyl Tert-Butyl Ether	Diethyl Phthalate	333.2	1.56	1.39	-10.9%	1.04	-33.3%	[39]
Methyl Tert-Butyl Ether	Dimethyl Carbonate	298.2	2.43	3.00	23.4%	M.G.	N.A.	248
Methyl Tert-Butyl Ether	Epsilon-Caprolactone	303.2	3.25	3.72	14.5%	M.G.	N.A.	[41]
Methyl Tert-Butyl Ether	Epsilon-Caprolactone	318.2	3.23	3.37	4.3%	M.G.	N.A.	[41]
Methyl Tert-Butyl Ether	Epsilon-Caprolactone	333.2	3.18	3.09	-2.8%	M.G.	N.A.	[41]
Methyl Tert-Butyl Ether	Ethyl Benzoate	313.2	1.34	1.26	-6.0%	1.05	-21.6%	[41]
Methyl Tert-Butyl Ether	Ethyl Benzoate	323.2	1.35	1.25	-7.4%	1.04	-23.0%	[41]
Methyl Tert-Butyl Ether	Ethyl Benzoate	333.2	1.36	1.24	-8.8%	1.04	-23.5%	[41]
Methyl Tert-Butyl Ether	Ethyl Benzoate	343.2	1.37	1.23	-10.2%	1.05	-23.4%	[41]
Methyl Tert-Butyl Ether	Glutaronitrile	303.2	6.69	9.14	36.6%	14.10	110.8%	[39]
Methyl Tert-Butyl Ether	Glutaronitrile	313.2	6.62	8.11	22.5%	13.68	106.6%	[39]
Methyl Tert-Butyl Ether	Glutaronitrile	323.2	6.59	7.26	10.2%	13.23	100.8%	[39]
Methyl Tert-Butyl Ether	Glutaronitrile	333.2	6.51	6.56	0.8%	12.77	96.2%	[39]
Methyl Tert-Butyl Ether	Methylcyclohexane	313.2	1.38	1.35	-2.2%	1.28	-7.2%	[56]
Methyl Tert-Butyl Ether	Methylcyclohexane	333.2	1.29	1.31	1.6%	1.23	-4.7%	[56]
Methyl Tert-Butyl Ether	N,N-Dibutylformamide	302.8	1.42	1.29	-9.0%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N,N-Dibutylformamide	318.3	1.38	1.26	-8.7%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N,N-Dibutylformamide	332.4	1.35	1.23	-8.9%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N,N-Diethylacetamide	303.2	1.90	1.87	-1.6%	1.37	-27.9%	[39]
Methyl Tert-Butyl Ether	N,N-Diethylacetamide	313.2	1.88	1.81	-3.7%	1.41	-25.0%	[39]
Methyl Tert-Butyl Ether	N,N-Diethylacetamide	323.2	1.88	1.76	-6.4%	1.45	-22.9%	[39]
Methyl Tert-Butyl Ether	N,N-Diethylacetamide	333.2	1.86	1.71	-8.1%	1.49	-19.9%	[39]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methyl Tert-Butyl Ether	N,N-Dimethylacetamide	303.6	2.90	3.09	6.6%	2.93	1.0%	[13]
Methyl Tert-Butyl Ether	N,N-Dimethylacetamide	317.6	2.47	2.86	15.6%	3.00	21.3%	[13]
Methyl Tert-Butyl Ether	N,N-Dimethylacetamide	333.0	2.10	2.64	25.7%	3.08	46.7%	[13]
Methyl Tert-Butyl Ether	N-Ethylacetamide	303.2	3.22	2.97	-7.8%	M.G.	N.A.	[39]
Methyl Tert-Butyl Ether	N-Ethylacetamide	313.2	3.22	2.90	-9.9%	M.G.	N.A.	[39]
Methyl Tert-Butyl Ether	N-Ethylacetamide	323.2	3.21	2.82	-12.1%	M.G.	N.A.	[39]
Methyl Tert-Butyl Ether	N-Ethylacetamide	333.2	3.21	2.74	-14.6%	M.G.	N.A.	[39]
Methyl Tert-Butyl Ether	N-Heptane	313.2	1.31	1.29	-1.5%	1.25	-4.6%	[56]
Methyl Tert-Butyl Ether	N-Heptane	323.2	1.22	1.27	4.1%	1.23	0.8%	[56]
Methyl Tert-Butyl Ether	N-Hexadecane	298.2	1.10	1.07	-3.0%	1.13	2.4%	[6]
Methyl Tert-Butyl Ether	N-Hexane	303.2	1.26	1.33	5.6%	1.28	1.6%	[56]
Methyl Tert-Butyl Ether	N-Hexane	323.2	1.20	1.29	7.5%	1.24	3.3%	[56]
Methyl Tert-Butyl Ether	N-Methylacetamide	303.3	4.78	4.07	-14.8%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N-Methylacetamide	318.4	4.44	3.86	-13.1%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N-Methylacetamide	333.2	4.18	3.65	-12.7%	M.P.	N.A.	[13]
Methyl Tert-Butyl Ether	N-Methylformamide	303.2	6.82	7.07	3.7%	M.P.	N.A.	[35]
Methyl Tert-Butyl Ether	N-Methylformamide	313.2	6.77	6.63	-2.1%	M.P.	N.A.	[35]
Methyl Tert-Butyl Ether	N-Methylformamide	323.2	6.72	6.20	-7.7%	M.P.	N.A.	[35]
Methyl Tert-Butyl Ether	N-Methylformamide	333.2	6.67	5.80	-13.0%	M.P.	N.A.	[35]
Methyl Tert-Butyl Ether	Sulfolane	303.8	7.32	9.16	25.2%	M.G.	N.A.	[13]
Methyl Tert-Butyl Ether	Sulfolane	317.9	7.16	7.74	8.2%	M.G.	N.A.	[13]
Methyl Tert-Butyl Ether	Sulfolane	333.6	6.89	6.56	-4.8%	M.G.	N.A.	[13]
Methyl Tert-Butyl Ether	Tetraethylene Glycol DME	303.2	1.52	1.54	1.3%	1.10	-27.6%	[7]
Methyl Tert-Butyl Ether	Tetraethylene Glycol DME	323.2	1.46	1.47	0.5%	1.08	-26.1%	[7]
Methyl Tert-Butyl Ether	Tetraethylene Glycol DME	343.2	1.40	1.40	0.4%	1.07	-23.3%	[7]
Methylcyclohexane	1,2-Dichloroethane	354.7	2.61	2.75	5.4%	2.23	-14.6%	[12]
Methylcyclohexane	1-Octanol	293.4	2.29	2.91	27.1%	2.39	4.4%	[31]
Methylcyclohexane	1-Octanol	303.5	2.29	2.79	21.8%	2.34	2.2%	[31]
Methylcyclohexane	1-Octanol	313.6	2.16	2.68	24.1%	2.30	6.5%	[31]
Methylcyclohexane	1-Octanol	323.4	2.10	2.57	22.4%	2.25	7.1%	[31]
Methylcyclohexane	2-Nitropropane	293.2	6.80	7.91	16.3%	5.88	-13.5%	[10]
Methylcyclohexane	2-Pyrrolidone	303.2	31.89	37.66	18.1%	M.G.	N.A.	[35]
Methylcyclohexane	2-Pyrrolidone	313.2	29.39	31.56	7.4%	M.G.	N.A.	[35]
Methylcyclohexane	2-Pyrrolidone	323.2	27.29	26.74	-2.0%	M.G.	N.A.	[35]
Methylcyclohexane	2-Pyrrolidone	333.2	25.38	22.89	-9.8%	M.G.	N.A.	[35]
Methylcyclohexane	Acetophenone	293.2	4.63	5.57	20.3%	7.62	64.6%	[10]
Methylcyclohexane	Aniline	293.2	17.53	18.49	5.5%	15.58	-11.1%	[37]
Methylcyclohexane	Aniline	293.2	17.50	18.49	5.7%	15.58	-11.0%	[10]
Methylcyclohexane	Benzyl Alcohol	298.2	8.05	10.50	30.4%	9.52	18.3%	[67]
Methylcyclohexane	Ethanol	313.2	10.75	12.22	13.7%	9.49	-11.7%	[79]
Methylcyclohexane	Ethanol	333.2	9.76	10.88	11.5%	8.48	-13.1%	[79]
Methylcyclohexane	Ethyl Benzoate	313.2	2.36	2.55	8.1%	M.G.	N.A.	[41]
Methylcyclohexane	Ethyl Benzoate	323.2	2.28	2.44	7.0%	M.G.	N.A.	[41]
Methylcyclohexane	Ethyl Benzoate	333.2	2.21	2.33	5.4%	M.G.	N.A.	[41]
Methylcyclohexane	Ethyl Benzoate	343.2	2.14	2.24	4.7%	M.G.	N.A.	[41]
Methylcyclohexane	Isopropanol	323.9	6.02	6.50	8.0%	4.82	-19.9%	[17]
Methylcyclohexane	Isopropanol	332.7	5.80	6.23	7.4%	4.65	-19.8%	[17]
Methylcyclohexane	Isopropanol	343.8	5.46	5.89	7.9%	4.44	-18.7%	[17]
Methylcyclohexane	Isopropanol	354.6	5.16	5.57	7.9%	4.24	-17.8%	[17]
Methylcyclohexane	Methyl Ethyl Ketone	314.7	3.80	3.86	1.6%	3.57	-6.1%	[12]
Methylcyclohexane	Methyl Ethyl Ketone	333.3	3.35	3.44	2.7%	3.20	-4.5%	[12]
Methylcyclohexane	Methyl Ethyl Ketone	348.6	3.08	3.17	2.9%	2.93	-4.9%	[12]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methylcyclohexane	Methyl Tert-Butyl Ether	313.2	0.96	1.37	42.7%	1.30	35.4%	[56]
Methylcyclohexane	Methyl Tert-Butyl Ether	333.2	0.99	1.33	34.3%	1.24	25.3%	[56]
Methylcyclohexane	N,N-Dibutylformamide	302.8	2.31	2.86	23.9%	2.33	0.9%	[13]
Methylcyclohexane	N,N-Dibutylformamide	318.3	2.15	2.62	22.0%	2.20	2.4%	[13]
Methylcyclohexane	N,N-Dibutylformamide	332.4	2.02	2.44	20.7%	2.09	3.4%	[13]
Methylcyclohexane	N,N-Dimethylacetamide	303.2	8.26	8.93	8.1%	7.19	-13.0%	[13]
Methylcyclohexane	N,N-Dimethylacetamide	317.6	7.44	7.61	2.3%	6.40	-14.0%	[13]
Methylcyclohexane	N,N-Dimethylacetamide	333.2	6.84	6.53	-4.6%	5.69	-16.8%	[13]
Methylcyclohexane	N-Formylmorpholine	313.3	22.80	25.18	10.4%	M.G.	N.A.	[43]
Methylcyclohexane	N-Formylmorpholine	332.7	18.50	18.75	1.4%	M.G.	N.A.	[43]
Methylcyclohexane	N-Formylmorpholine	352.5	15.60	14.43	-7.5%	M.G.	N.A.	[43]
Methylcyclohexane	N-Formylmorpholine	373.4	13.20	11.36	-13.9%	M.G.	N.A.	[43]
Methylcyclohexane	Nitrobenzene	293.2	7.22	7.01	-2.9%	6.41	-11.2%	[10]
Methylcyclohexane	Nitromethane	343.2	28.00	19.46	-30.5%	27.74	-0.9%	[83]
Methylcyclohexane	Nitromethane	353.2	24.90	16.54	-33.6%	24.59	-1.2%	[83]
Methylcyclohexane	N-Methyl-2-Pyrrolidone	323.4	9.67	7.87	-18.6%	7.26	-24.9%	[43]
Methylcyclohexane	N-Methyl-2-Pyrrolidone	333.2	9.14	7.16	-21.7%	6.75	-26.1%	[43]
Methylcyclohexane	N-Methyl-2-Pyrrolidone	343.4	8.64	6.54	-24.3%	6.26	-27.5%	[43]
Methylcyclohexane	N-Methylacetamide	303.1	12.01	13.88	15.6%	10.42	-13.2%	[13]
Methylcyclohexane	N-Methylacetamide	318.4	11.07	12.45	12.5%	9.86	-10.9%	[13]
Methylcyclohexane	N-Methylacetamide	333.2	10.64	11.14	4.7%	9.37	-11.9%	[13]
Methylcyclohexane	N-Methylformamide	303.2	31.15	36.88	18.4%	M.P.	N.A.	[35]
Methylcyclohexane	N-Methylformamide	313.2	29.45	32.72	11.1%	M.P.	N.A.	[35]
Methylcyclohexane	N-Methylformamide	323.2	27.91	29.00	3.9%	M.P.	N.A.	[35]
Methylcyclohexane	N-Methylformamide	333.2	26.69	25.71	-3.7%	M.P.	N.A.	[35]
Methylcyclohexane	Phenol	323.2	10.20	11.18	9.6%	6.67	-34.6%	[10]
Methylcyclohexane	Phenol	328.2	10.57	10.84	2.6%	6.48	-38.7%	[14]
Methylcyclohexane	Phenol	343.2	9.44	9.85	4.3%	5.97	-36.8%	[14]
Methylcyclohexane	Phenol	358.2	8.65	8.91	3.0%	5.57	-35.6%	[14]
Methylcyclohexane	Phenol	373.2	8.45	8.04	-4.9%	5.24	-38.0%	[14]
Methylcyclohexane	Quinoline	293.2	6.60	6.39	-3.2%	M.G.	N.A.	[37]
Methylcyclohexane	Sulfolane	303.6	38.71	41.45	7.1%	M.G.	N.A.	[13]
Methylcyclohexane	Sulfolane	317.9	32.37	30.90	-4.5%	M.G.	N.A.	[13]
Methylcyclohexane	Sulfolane	332.8	24.94	23.62	-5.3%	M.G.	N.A.	[13]
Methylcyclohexane	Toluene	343.2	1.38	1.43	3.6%	1.36	-1.4%	[83]
Methylcyclohexane	Toluene	353.2	1.36	1.40	2.9%	1.34	-1.5%	[83]
Methylcyclohexane	Tributyl Phosphate	298.6	1.65	1.96	18.8%	M.G.	N.A.	[27]
Methylcyclohexane	Tributyl Phosphate	302.9	1.63	1.92	17.8%	M.G.	N.A.	[27]
Methylcyclohexane	Tributyl Phosphate	308.6	1.62	1.86	14.8%	M.G.	N.A.	[27]
Methylcyclohexane	Tributyl Phosphate	313.1	1.60	1.82	13.8%	M.G.	N.A.	[27]
Methylcyclohexane	Tributyl Phosphate	323.7	1.49	1.74	16.8%	M.G.	N.A.	[27]
Methylcyclohexane	Tributyl Phosphate	330.0	1.40	1.70	21.4%	M.G.	N.A.	[27]
Methylcyclopentane	1-Pentanol	303.5	3.36	3.58	6.5%	2.90	-13.7%	[33]
Methylcyclopentane	1-Pentanol	313.2	3.28	3.48	6.1%	2.85	-13.1%	[33]
Methylcyclopentane	1-Pentanol	323.5	3.21	3.38	5.3%	2.78	-13.4%	[33]
Methylcyclopentane	2-Pyrrolidone	303.2	24.93	25.66	2.9%	M.G.	N.A.	[35]
Methylcyclopentane	2-Pyrrolidone	313.2	23.12	21.96	-5.0%	M.G.	N.A.	[35]
Methylcyclopentane	2-Pyrrolidone	323.2	21.53	18.97	-11.9%	M.G.	N.A.	[35]
Methylcyclopentane	2-Pyrrolidone	333.2	20.03	16.55	-17.4%	M.G.	N.A.	[35]
Methylcyclopentane	Acetone	308.2	5.62	5.81	3.4%	4.16	-26.0%	[75]
Methylcyclopentane	Aniline	293.2	13.70	13.46	-1.8%	10.40	-24.1%	[37]
Methylcyclopentane	Ethanol	313.2	8.03	9.87	22.9%	6.90	-14.1%	[75]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Methylcyclopentane	Ethyl Acetate	303.2	2.87	3.11	8.4%	3.01	4.9%	[75]
Methylcyclopentane	Ethyl Benzoate	313.2	2.21	2.24	1.4%	M.G.	N.A.	[41]
Methylcyclopentane	Ethyl Benzoate	323.2	2.15	2.15	0.0%	M.G.	N.A.	[41]
Methylcyclopentane	Ethyl Benzoate	333.2	2.11	2.07	-1.9%	M.G.	N.A.	[41]
Methylcyclopentane	Ethyl Benzoate	343.2	2.07	2.00	-3.4%	M.G.	N.A.	[41]
Methylcyclopentane	N-Formylmorpholine	313.3	17.50	17.53	0.2%	M.G.	N.A.	[43]
Methylcyclopentane	N-Formylmorpholine	332.7	14.20	13.51	-4.9%	M.G.	N.A.	[43]
Methylcyclopentane	N-Formylmorpholine	352.5	12.50	10.73	-14.2%	M.G.	N.A.	[43]
Methylcyclopentane	N-Formylmorpholine	373.4	10.70	8.69	-18.8%	M.G.	N.A.	[43]
Methylcyclopentane	N-Methyl-2-Pyrrolidone	323.4	8.41	6.28	-25.3%	5.11	-39.2%	[43]
Methylcyclopentane	N-Methyl-2-Pyrrolidone	333.2	7.92	5.78	-27.0%	4.81	-39.3%	[43]
Methylcyclopentane	N-Methyl-2-Pyrrolidone	343.4	7.50	5.33	-28.9%	4.51	-39.9%	[43]
Methylcyclopentane	N-Methylformamide	303.2	24.30	25.99	7.0%	M.P.	N.A.	[35]
Methylcyclopentane	N-Methylformamide	313.2	22.95	23.39	1.9%	M.P.	N.A.	[35]
Methylcyclopentane	N-Methylformamide	323.2	21.82	21.03	-3.6%	M.P.	N.A.	[35]
Methylcyclopentane	N-Methylformamide	333.2	20.75	18.91	-8.9%	M.P.	N.A.	[35]
Methylcyclopentane	Phenol	328.2	9.36	8.43	-9.9%	5.05	-46.0%	[14]
Methylcyclopentane	Phenol	343.2	8.27	7.75	-6.3%	4.71	-43.0%	[14]
Methylcyclopentane	Phenol	358.2	7.70	7.09	-7.9%	4.43	-42.5%	[14]
Methylcyclopentane	Phenol	373.2	7.64	6.48	-15.2%	4.19	-45.2%	[14]
N,N-Dimethylacetamide	N-Hexadecane	298.2	26.08	20.74	-20.5%	7.29	-72.0%	[6]
N,N-Dimethylformamide	1-Propanol	313.2	0.85	1.26	47.4%	0.79	-7.6%	67
N,N-Dimethylformamide	Cyclohexane	313.2	28.80	26.57	-7.7%	19.95	-30.7%	[42]
N,N-Dimethylformamide	Cyclohexane	333.2	19.20	18.16	-5.4%	13.98	-27.2%	[42]
N,N-Dimethylformamide	Cyclohexane	333.2	19.00	18.16	-4.4%	13.98	-26.4%	[42]
N,N-Dimethylformamide	Ethanol	313.2	0.82	1.05	28.0%	0.72	-12.2%	66
N,N-Dimethylformamide	Ethyl Acetate	313.2	1.90	2.09	10.3%	2.03	7.1%	80
N,N-Dimethylformamide	Ethyl Acetate	333.2	1.84	1.92	4.6%	1.95	6.3%	80
N,N-Dimethylformamide	Isopropanol	353.2	0.87	1.52	75.6%	0.71	-18.0%	276
N,N-Dimethylformamide	Methanol	313.2	0.63	0.50	-20.9%	0.57	-9.8%	65
N,N-Dimethylformamide	N-Decane	293.2	30.20	36.09	19.5%	23.03	-23.7%	[42]
N,N-Dimethylformamide	N-Decane	313.2	21.60	22.62	4.7%	17.26	-20.1%	[42]
N,N-Dimethylformamide	N-Decane	333.2	15.50	15.38	-0.8%	13.36	-13.8%	[42]
N,N-Dimethylformamide	N-Hexadecane	298.2	24.48	27.40	11.9%	16.08	-34.3%	[6]
N,N-Dimethylformamide	N-Hexane	303.2	32.30	32.48	0.6%	27.23	-15.7%	[42]
N,N-Dimethylformamide	N-Hexane	303.2	33.00	32.48	-1.6%	27.23	-17.5%	[42]
N,N-Dimethylformamide	N-Hexane	313.2	27.40	26.05	-4.9%	23.68	-13.6%	[42]
N,N-Dimethylformamide	N-Hexane	313.2	27.10	26.05	-3.9%	23.68	-12.6%	[42]
N,N-Dimethylformamide	N-Nonane	313.2	22.10	23.30	5.4%	18.39	-16.8%	[42]
N,N-Dimethylformamide	N-Octane	313.2	22.70	24.09	6.1%	19.76	-13.0%	[42]
N-Butane	Aniline	293.2	15.11	12.70	-15.9%	12.84	-15.0%	[37]
N-Butane	Benzyl Alcohol	298.2	9.55	8.10	-15.2%	7.00	-26.7%	[67]
N-Butane	Quinoline	293.2	6.96	5.73	-17.7%	M.G.	N.A.	[37]
N-Butylbenzene	Acetonitrile	298.2	11.10	10.76	-3.1%	10.43	-6.0%	[63]
N-Butylbenzene	Acetonitrile	298.2	11.10	10.76	-3.1%	10.43	-6.0%	[64]
N-Butylbenzene	Isopropanol	298.2	8.51	8.42	-1.1%	6.74	-20.8%	[63]
N-Butylbenzene	Isopropanol	298.2	8.50	8.42	-0.9%	6.74	-20.7%	[64]
N-Butylbenzene	Methanol	298.2	24.50	25.41	3.7%	24.30	-0.8%	[63]
N-Butylbenzene	Methanol	298.2	24.80	25.41	2.5%	24.30	-2.0%	[64]
N-Butylbenzene	Tetrahydrofuran	298.2	0.90	0.99	10.0%	0.82	-8.9%	[63]
N-Butylbenzene	Tetrahydrofuran	298.2	0.90	0.99	10.0%	0.82	-8.9%	[64]
N-Decane	Acetone	313.2	12.32	11.03	-10.4%	9.23	-25.1%	317

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
N-Decane	Acetone	333.2	8.74	8.50	-2.7%	7.22	-17.4%	317
N-Decane	Carbon Tetrachloride	313.2	1.10	1.06	-3.9%	1.11	0.6%	92
N-Decane	N-Formylmorpholine	313.3	90.10	113.48	25.9%	M.G.	N.A.	[43]
N-Decane	N-Formylmorpholine	332.7	65.80	72.28	9.8%	M.G.	N.A.	[43]
N-Decane	N-Formylmorpholine	352.5	53.30	48.44	-9.1%	M.G.	N.A.	[43]
N-Decane	N-Formylmorpholine	373.4	42.20	33.57	-20.5%	M.G.	N.A.	[43]
N-Decane	N-Hexadecane	298.2	1.09	0.95	-12.8%	0.97	-11.0%	[6]
N-Decane	Phenol	418.2	8.88	12.16	36.9%	7.98	-10.2%	44
N-Decane	Phenol	433.2	8.20	10.55	28.7%	6.44	-21.4%	44
N-Decane	P-Xylene	313.2	1.31	1.41	7.8%	1.20	-8.3%	100
N-Dodecane	Tributyl Phosphate	363.2	2.45	3.47	41.6%	M.G.	N.A.	[20]
N-Dodecane	Tributyl Phosphate	373.2	2.42	3.28	35.5%	M.G.	N.A.	[20]
N-Dodecane	Tributyl Phosphate	383.2	2.42	3.12	28.9%	M.G.	N.A.	[20]
N-Heptane	1,2-Dichloroethane	298.2	5.80	4.96	-14.5%	4.01	-30.9%	[50]
N-Heptane	1,2-Dichloroethane	318.5	4.45	4.15	-6.7%	3.27	-26.5%	[12]
N-Heptane	1,2-Dichloroethane	337.2	3.86	3.61	-6.5%	2.75	-28.8%	[12]
N-Heptane	1,2-Dichloroethane	354.2	3.10	3.23	4.2%	2.38	-23.2%	[12]
N-Heptane	1,4-Dioxane	298.2	5.96	5.48	-8.1%	6.53	9.5%	33
N-Heptane	1,4-Dioxane	298.2	7.61	5.48	-28.0%	6.53	-14.2%	[50]
N-Heptane	1,4-Dioxane	303.2	5.78	5.24	-9.3%	6.21	7.5%	33
N-Heptane	1,4-Dioxane	308.2	6.10	5.03	-17.6%	5.91	-3.1%	33
N-Heptane	1,4-Dioxane	313.2	6.14	4.83	-21.3%	5.64	-8.2%	33
N-Heptane	1,4-Dioxane	313.4	5.47	4.82	-11.9%	5.63	2.9%	[19]
N-Heptane	1,4-Dioxane	333.2	4.83	4.16	-13.9%	4.73	-2.1%	[19]
N-Heptane	1,4-Dioxane	353.2	4.13	3.66	-11.3%	4.03	-2.4%	33
N-Heptane	1,4-Dioxane	353.2	3.97	3.66	-7.8%	4.03	1.5%	[19]
N-Heptane	1,5-Dimethyl-2-Pyrrolidinone	298.2	9.36	10.13	8.2%	M.G.	N.A.	[29]
N-Heptane	1,5-Dimethyl-2-Pyrrolidinone	308.2	8.98	9.03	0.6%	M.G.	N.A.	[29]
N-Heptane	1,5-Dimethyl-2-Pyrrolidinone	318.2	8.63	8.13	-5.8%	M.G.	N.A.	[29]
N-Heptane	1-Butanol	293.2	7.00	6.13	-12.4%	5.48	-21.7%	[10]
N-Heptane	1-Butanol	298.2	5.86	6.04	3.1%	5.43	-7.3%	[50]
N-Heptane	1-Butanol	308.2	5.55	5.84	5.2%	5.31	-4.3%	[30]
N-Heptane	1-Butanol	318.2	5.39	5.62	4.3%	5.17	-4.1%	[30]
N-Heptane	1-Butanol	328.2	5.21	5.39	3.5%	5.00	-4.0%	[30]
N-Heptane	1-Butanol	333.2	5.08	5.26	3.6%	4.91	-3.3%	144
N-Heptane	1-Butanol	353.2	5.13	4.78	-6.8%	4.50	-12.3%	[21]
N-Heptane	1-Butanol	363.2	4.54	4.54	-0.1%	4.26	-6.2%	144
N-Heptane	1-Butanol	373.2	4.76	4.32	-9.2%	4.02	-15.5%	[21]
N-Heptane	1-Ethylpyrrolidin-2-One	298.2	9.94	10.01	0.7%	4.91	-50.6%	[29]
N-Heptane	1-Ethylpyrrolidin-2-One	308.2	8.88	8.94	0.7%	4.68	-47.3%	[29]
N-Heptane	1-Ethylpyrrolidin-2-One	318.2	8.03	8.06	0.4%	4.46	-44.5%	[29]
N-Heptane	1-Hexene	298.2	1.14	0.99	-13.2%	1.05	-7.9%	[50]
N-Heptane	1-Octanol	293.4	2.90	3.28	13.1%	2.79	-3.8%	[31]
N-Heptane	1-Octanol	298.2	3.05	3.21	5.2%	2.77	-9.2%	[2]
N-Heptane	1-Octanol	298.2	3.00	3.21	7.0%	2.77	-7.7%	[50]
N-Heptane	1-Octanol	298.2	3.06	3.21	4.9%	2.77	-9.5%	[32]
N-Heptane	1-Octanol	298.2	3.05	3.21	5.2%	2.77	-9.2%	[4]
N-Heptane	1-Octanol	303.5	2.92	3.13	7.2%	2.75	-5.8%	[31]
N-Heptane	1-Octanol	308.2	3.07	3.07	0.0%	2.74	-10.7%	[2]
N-Heptane	1-Octanol	313.6	2.89	2.99	3.5%	2.71	-6.2%	[31]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
N-Heptane	1-Octanol	323.2	2.97	2.87	-3.4%	2.66	-10.4%	[2]
N-Heptane	1-Octanol	323.4	2.71	2.86	5.5%	2.66	-1.8%	[31]
N-Heptane	1-Octene	298.2	1.05	1.01	-3.8%	1.06	1.0%	[50]
N-Heptane	1-Pentanol	303.5	4.63	4.81	3.9%	4.26	-8.0%	[33]
N-Heptane	1-Pentanol	308.2	4.70	4.74	0.9%	4.22	-10.2%	[30]
N-Heptane	1-Pentanol	313.2	4.73	4.65	-1.7%	4.18	-11.6%	[33]
N-Heptane	1-Pentanol	318.2	4.61	4.57	-0.9%	4.13	-10.4%	[30]
N-Heptane	1-Pentanol	323.5	4.43	4.47	0.9%	4.07	-8.1%	[33]
N-Heptane	1-Pentanol	328.2	4.70	4.39	-6.6%	4.02	-14.5%	[30]
N-Heptane	1-Phenyl-1-Butanone	298.1	4.06	4.36	7.4%	4.20	3.4%	[34]
N-Heptane	1-Propanol	298.2	7.91	7.84	-0.9%	7.51	-5.1%	[50]
N-Heptane	1-Propanol	303.2	7.41	7.73	4.4%	7.41	0.1%	309
N-Heptane	1-Propanol	308.2	7.35	7.61	3.5%	7.30	-0.7%	[47]
N-Heptane	1-Propanol	313.2	7.14	7.47	4.7%	7.18	0.6%	309
N-Heptane	1-Propanol	323.2	6.85	7.17	4.7%	6.91	0.9%	309
N-Heptane	1-Propanol	333.2	6.61	6.84	3.5%	6.61	0.0%	309
N-Heptane	1-Propanol	333.2	6.34	6.84	7.9%	6.61	4.3%	[21]
N-Heptane	1-Propanol	353.2	5.89	6.15	4.4%	5.90	0.2%	[21]
N-Heptane	2,2,4-Trimethylpentane	298.2	1.07	1.07	0.0%	1.00	-6.5%	[50]
N-Heptane	2-Heptanone	298.2	2.41	2.43	0.8%	2.65	10.0%	[50]
N-Heptane	2-Methyl-2-Propanol	313.2	4.01	4.91	22.4%	3.33	-17.0%	1
N-Heptane	2-Nitropropane	293.2	8.81	9.12	3.5%	6.39	-27.5%	[10]
N-Heptane	2-Pentanone	298.2	3.33	3.47	4.2%	3.78	13.5%	[50]
N-Heptane	2-Pyrrolidone	303.2	55.32	66.36	20.0%	M.G.	N.A.	[35]
N-Heptane	2-Pyrrolidone	313.2	49.82	53.99	8.4%	M.G.	N.A.	[35]
N-Heptane	2-Pyrrolidone	323.2	45.54	44.49	-2.3%	M.G.	N.A.	[35]
N-Heptane	2-Pyrrolidone	333.2	41.92	37.12	-11.5%	M.G.	N.A.	[35]
N-Heptane	Acetic Acid	298.2	22.52	19.79	-12.1%	14.31	-36.5%	[50]
N-Heptane	Acetone	273.2	13.69	10.81	-21.0%	9.23	-32.6%	318
N-Heptane	Acetone	298.2	8.45	7.78	-7.9%	7.12	-15.7%	[50]
N-Heptane	Acetone	303.2	7.63	7.34	-3.8%	6.78	-11.1%	[18]
N-Heptane	Acetone	303.2	7.81	7.34	-6.0%	6.78	-13.2%	[18]
N-Heptane	Acetone	313.2	7.35	6.59	-10.3%	6.16	-16.2%	[18]
N-Heptane	Acetone	313.2	7.33	6.59	-10.1%	6.16	-16.0%	[18]
N-Heptane	Acetone	323.2	6.60	5.97	-9.6%	5.63	-14.7%	318
N-Heptane	Acetonitrile	298.2	31.60	39.02	23.5%	33.09	4.7%	[36]
N-Heptane	Acetonitrile	298.2	39.55	39.02	-1.3%	33.09	-16.3%	[50]
N-Heptane	Acetophenone	293.2	7.58	7.43	-2.0%	11.93	57.4%	[10]
N-Heptane	Acetophenone	298.2	7.36	7.02	-4.6%	11.38	54.6%	[50]
N-Heptane	Alpha-Pinene	353.2	1.16	1.25	7.8%	1.50	29.3%	[22]
N-Heptane	Alpha-Pinene	373.2	1.19	1.24	4.2%	1.50	26.1%	[22]
N-Heptane	Aniline	293.2	31.77	29.48	-7.2%	28.83	-9.3%	[37]
N-Heptane	Aniline	293.2	31.80	29.48	-7.3%	28.83	-9.3%	[10]
N-Heptane	Anisole	293.2	4.25	4.20	-1.2%	3.09	-27.3%	[10]
N-Heptane	Anisole	298.2	4.16	4.03	-3.1%	3.00	-27.9%	[50]
N-Heptane	Anisole	358.2	2.73	2.78	1.7%	2.21	-19.1%	55
N-Heptane	Anisole	368.2	2.59	2.65	2.3%	2.11	-18.5%	55
N-Heptane	Benzene	298.2	2.06	2.11	2.4%	2.14	3.9%	[50]
N-Heptane	Benzene	313.2	1.97	1.97	0.0%	1.97	0.0%	104
N-Heptane	Benzene	318.0	1.92	1.93	0.5%	1.93	0.5%	[12]
N-Heptane	Benzene	333.2	1.80	1.82	1.1%	1.79	-0.6%	104
N-Heptane	Benzene	335.4	1.71	1.81	5.8%	1.77	3.5%	[12]

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N-Heptane	Benzene	349.4	1.59	1.73	8.8%	1.67	5.0%	[12]
N-Heptane	Benzonitrile	293.2	7.53	8.26	9.7%	M.G.	N.A.	[10]
N-Heptane	Benzonitrile	298.2	7.18	7.79	8.5%	M.G.	N.A.	[50]
N-Heptane	Benzyl Alcohol	298.2	16.70	15.72	-5.9%	11.93	-28.6%	[50]
N-Heptane	Butyl Acetate	298.2	2.48	2.35	-5.2%	3.10	25.0%	[50]
N-Heptane	Butyl Ether	293.2	1.00	1.18	18.0%	1.09	9.0%	[5]
N-Heptane	Butyronitrile	298.2	7.76	7.70	-0.8%	6.53	-15.9%	[50]
N-Heptane	Carbon Disulfide	298.2	2.24	2.18	-2.7%	2.27	1.3%	[50]
N-Heptane	Carbon Tetrachloride	298.2	1.34	1.29	-3.7%	1.29	-3.7%	[50]
N-Heptane	Carbon Tetrachloride	313.2	1.24	1.26	1.8%	1.24	0.2%	94
N-Heptane	Carbon Tetrachloride	328.3	1.27	1.23	-3.1%	1.21	-4.7%	[12]
N-Heptane	Carbon Tetrachloride	349.1	1.15	1.20	4.3%	1.17	1.7%	[12]
N-Heptane	Chlorobenzene	298.2	2.22	2.22	0.0%	2.64	18.9%	[50]
N-Heptane	Chloroform	298.2	2.06	2.15	4.4%	1.99	-3.4%	[50]
N-Heptane	Chloroform	323.2	1.68	1.90	12.8%	1.76	4.5%	321
N-Heptane	Cyclohexane	298.2	1.13	1.10	-2.7%	1.07	-5.3%	[50]
N-Heptane	Cyclohexanone	298.2	4.83	4.66	-3.5%	3.34	-30.8%	[50]
N-Heptane	Dichloromethane	298.2	3.44	3.50	1.7%	3.14	-8.7%	[50]
N-Heptane	Diethyl Phthalate	303.2	5.74	6.00	4.5%	M.G.	N.A.	[39]
N-Heptane	Diethyl Phthalate	313.2	5.33	5.47	2.6%	M.G.	N.A.	[39]
N-Heptane	Diethyl Phthalate	323.2	5.07	5.03	-0.8%	M.G.	N.A.	[39]
N-Heptane	Diethyl Phthalate	333.2	4.76	4.65	-2.3%	M.G.	N.A.	[39]
N-Heptane	Diisopropyl Ether	313.2	1.08	1.22	13.0%	1.07	-0.9%	[56]
N-Heptane	Diisopropyl Ether	323.2	1.06	1.21	14.1%	1.06	0.0%	283
N-Heptane	Diisopropyl Ether	333.2	1.02	1.20	17.6%	1.06	3.9%	[56]
N-Heptane	Diisopropyl Ether	343.2	1.05	1.19	13.4%	1.05	0.0%	283
N-Heptane	Dimethyl Carbonate	283.2	15.59	12.63	-19.0%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	293.2	12.71	11.07	-12.9%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	313.2	9.11	8.77	-3.7%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	323.2	7.91	7.92	0.1%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	333.2	6.96	7.20	3.5%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	343.2	6.18	6.59	6.6%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	363.2	5.00	5.63	12.6%	M.G.	N.A.	241
N-Heptane	Dimethyl Carbonate	373.2	4.54	5.24	15.5%	M.G.	N.A.	241
N-Heptane	Dimethyl Sulfoxide	283.2	150.00	162.82	8.5%	160.10	6.7%	[40]
N-Heptane	Dimethyl Sulfoxide	298.2	108.22	101.40	-6.3%	111.07	2.6%	[50]
N-Heptane	Dimethyl Sulfoxide	313.2	105.00	67.24	-36.0%	79.08	-24.7%	[68]
N-Heptane	Di-N-Propyl Ether	343.2	1.10	1.95	77.7%	1.10	0.2%	305
N-Heptane	Epsilon-Caprolactone	303.2	16.00	17.13	7.1%	M.G.	N.A.	[41]
N-Heptane	Epsilon-Caprolactone	318.2	14.50	13.77	-5.0%	M.G.	N.A.	[41]
N-Heptane	Epsilon-Caprolactone	333.2	13.00	11.37	-12.5%	M.G.	N.A.	[41]
N-Heptane	Ethanol	293.5	12.70	15.24	20.0%	12.64	-0.5%	[28]
N-Heptane	Ethanol	298.2	13.07	15.00	14.8%	12.43	-4.9%	[50]
N-Heptane	Ethanol	303.2	13.13	14.70	11.9%	12.19	-7.2%	141
N-Heptane	Ethanol	303.2	15.00	14.70	-2.0%	12.19	-18.7%	[18]
N-Heptane	Ethanol	303.3	11.90	14.69	23.4%	12.19	2.4%	[28]
N-Heptane	Ethanol	303.3	13.11	14.69	12.1%	12.19	-7.0%	141
N-Heptane	Ethanol	313.1	11.10	14.00	26.1%	11.65	5.0%	[28]
N-Heptane	Ethanol	313.2	12.88	13.99	8.7%	11.64	-9.6%	141
N-Heptane	Ethanol	313.2	14.10	13.99	-0.8%	11.64	-17.4%	[18]
N-Heptane	Ethanol	313.2	15.34	13.99	-8.8%	11.64	-24.1%	[79]
N-Heptane	Ethanol	319.4	11.80	13.50	14.4%	11.27	-4.5%	[12]

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N-Heptane	Ethanol	322.2	12.00	13.27	10.6%	11.09	-7.6%	[48]
N-Heptane	Ethanol	322.8	10.50	13.22	25.9%	11.05	5.2%	[28]
N-Heptane	Ethanol	323.2	11.56	13.19	14.1%	11.02	-4.7%	141
N-Heptane	Ethanol	323.2	13.30	13.19	-0.8%	11.02	-17.1%	[18]
N-Heptane	Ethanol	333.2	14.21	12.34	-13.2%	10.33	-27.3%	[79]
N-Heptane	Ethanol	335.2	10.90	12.16	11.6%	10.18	-6.6%	[12]
N-Heptane	Ethanol	337.7	11.20	11.95	6.7%	10.00	-10.7%	[48]
N-Heptane	Ethanol	343.1	10.90	11.47	5.2%	9.59	-12.0%	141
N-Heptane	Ethanol	347.8	10.30	11.08	7.6%	9.23	-10.4%	[12]
N-Heptane	Ethanol	354.2	10.80	10.54	-2.4%	8.73	-19.2%	[48]
N-Heptane	Ethyl Acetate	298.2	3.82	3.74	-2.1%	3.83	0.3%	[50]
N-Heptane	Ethyl Acetate	323.2	3.22	3.18	-1.2%	3.15	-2.1%	153
N-Heptane	Ethyl Acetate	343.2	2.85	2.85	0.0%	2.75	-3.5%	153
N-Heptane	Ethyl Benzoate	313.2	3.16	3.20	1.3%	M.G.	N.A.	[41]
N-Heptane	Ethyl Benzoate	323.2	3.05	3.03	-0.7%	M.G.	N.A.	[41]
N-Heptane	Ethyl Benzoate	333.2	2.95	2.88	-2.4%	M.G.	N.A.	[41]
N-Heptane	Ethyl Benzoate	343.2	2.86	2.74	-4.2%	M.G.	N.A.	[41]
N-Heptane	Isopropanol	298.2	7.96	7.52	-5.5%	5.91	-25.8%	[50]
N-Heptane	Isopropanol	303.2	6.96	7.39	6.2%	5.84	-16.0%	308
N-Heptane	Isopropanol	308.2	8.50	7.25	-14.7%	5.75	-32.4%	[47]
N-Heptane	Isopropanol	323.9	6.54	6.77	3.5%	5.44	-16.8%	[17]
N-Heptane	Isopropanol	332.7	6.28	6.48	3.2%	5.24	-16.6%	[17]
N-Heptane	Isopropanol	343.8	5.90	6.11	3.6%	4.95	-16.1%	[17]
N-Heptane	Isopropanol	354.6	5.70	5.75	0.9%	4.64	-18.6%	[17]
N-Heptane	Methanol	298.2	35.14	39.13	11.4%	29.63	-15.7%	[50]
N-Heptane	Methanol	303.2	35.10	37.91	8.0%	28.73	-18.1%	[18]
N-Heptane	Methanol	313.2	31.70	35.14	10.9%	27.03	-14.7%	[18]
N-Heptane	Methyl Acetate	298.2	7.13	6.56	-8.0%	6.22	-12.8%	[50]
N-Heptane	Methyl Ethyl Ketone	298.2	4.22	4.65	10.2%	4.92	16.6%	[50]
N-Heptane	Methyl Ethyl Ketone	303.2	4.66	4.46	-4.3%	4.74	1.7%	[18]
N-Heptane	Methyl Ethyl Ketone	313.2	4.41	4.13	-6.3%	4.42	0.2%	[18]
N-Heptane	Methyl Ethyl Ketone	313.2	4.41	4.13	-6.3%	4.42	0.2%	[18]
N-Heptane	Methyl Ethyl Ketone	323.2	4.16	3.85	-7.5%	4.12	-1.0%	[18]
N-Heptane	Methyl Ethyl Ketone	333.1	3.93	3.61	-8.1%	3.86	-1.8%	[18]
N-Heptane	Methyl Ethyl Ketone	333.2	3.90	3.60	-7.7%	3.86	-1.0%	[18]
N-Heptane	Methyl Isobutyl Ketone	293.2	2.06	2.89	40.3%	3.17	53.9%	[5]
N-Heptane	Methyl Isobutyl Ketone	328.2	2.62	2.42	-7.6%	2.70	3.1%	[49]
N-Heptane	Methyl Isobutyl Ketone	348.2	2.35	2.23	-5.1%	2.49	6.0%	[49]
N-Heptane	Methyl Isobutyl Ketone	388.2	1.90	1.95	2.6%	2.16	13.7%	[49]
N-Heptane	Methyl Tert-Butyl Ether	313.2	1.01	1.35	33.7%	1.27	25.7%	[56]
N-Heptane	Methyl Tert-Butyl Ether	323.2	0.94	1.32	40.4%	1.25	33.0%	[56]
N-Heptane	N,N-Dibutylformamide	302.8	3.05	3.59	17.8%	3.06	0.4%	[13]
N-Heptane	N,N-Dibutylformamide	318.3	2.80	3.24	15.8%	2.94	5.1%	[13]
N-Heptane	N,N-Dibutylformamide	332.4	2.67	2.98	11.8%	2.85	6.9%	[13]
N-Heptane	N,N-Diethylacetamide	303.2	5.76	6.03	4.7%	2.38	-58.7%	[39]
N-Heptane	N,N-Diethylacetamide	313.2	5.35	5.52	3.2%	2.28	-57.4%	[39]
N-Heptane	N,N-Diethylacetamide	323.2	5.06	5.08	0.4%	2.20	-56.5%	[39]
N-Heptane	N,N-Diethylacetamide	333.2	4.74	4.71	-0.6%	2.13	-55.1%	[39]
N-Heptane	N,N-Dimethylacetamide	303.2	11.60	11.97	3.2%	9.38	-19.1%	[13]
N-Heptane	N,N-Dimethylacetamide	317.6	9.80	9.95	1.6%	8.13	-17.0%	[13]
N-Heptane	N,N-Dimethylacetamide	333.4	8.28	8.33	0.6%	7.08	-14.5%	[13]
N-Heptane	N,N-Dimethylformamide	283.2	30.00	27.29	-9.0%	24.15	-19.5%	[40]

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N-Heptane	N,N-Dimethylformamide	293.2	26.50	22.61	-14.7%	21.03	-20.6%	[10]
N-Heptane	N-Decane	298.2	0.98	0.98	0.0%	0.99	1.0%	[50]
N-Heptane	N-Dodecane	298.2	1.01	0.96	-5.0%	0.97	-4.0%	[50]
N-Heptane	N-Ethylacetamide	303.2	11.40	12.08	6.0%	M.G.	N.A.	[39]
N-Heptane	N-Ethylacetamide	313.2	11.00	11.26	2.4%	M.G.	N.A.	[39]
N-Heptane	N-Ethylacetamide	323.2	10.70	10.46	-2.2%	M.G.	N.A.	[39]
N-Heptane	N-Ethylacetamide	333.2	10.30	9.72	-5.6%	M.G.	N.A.	[39]
N-Heptane	N-Formylmorpholine	313.3	42.30	40.62	-4.0%	M.G.	N.A.	[43]
N-Heptane	N-Formylmorpholine	332.7	31.40	28.89	-8.0%	M.G.	N.A.	[43]
N-Heptane	N-Formylmorpholine	352.5	26.10	21.35	-18.2%	M.G.	N.A.	[43]
N-Heptane	N-Formylmorpholine	373.4	21.50	16.18	-24.7%	M.G.	N.A.	[43]
N-Heptane	N-Heptane	298.2	1.05	1.00	-4.8%	1.00	-4.8%	[50]
N-Heptane	N-Hexadecane	293.2	0.92	0.89	-3.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	298.2	0.92	0.89	-3.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	298.2	0.92	0.89	-3.3%	0.92	0.0%	[50]
N-Heptane	N-Hexadecane	298.2	0.92	0.89	-3.7%	0.92	-0.4%	[6]
N-Heptane	N-Hexadecane	303.2	0.92	0.89	-3.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	313.2	0.92	0.89	-3.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	323.2	0.92	0.88	-4.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	333.2	0.92	0.88	-4.3%	0.92	0.0%	[70]
N-Heptane	N-Hexadecane	393.2	0.88	0.88	0.0%	0.92	4.5%	[71]
N-Heptane	N-Hexadecane	453.2	0.87	0.87	0.0%	0.92	5.7%	[71]
N-Heptane	N-Hexane	298.2	0.97	1.00	3.1%	1.00	3.1%	[50]
N-Heptane	Nitrobenzene	293.2	9.40	9.40	0.0%	9.44	0.4%	[10]
N-Heptane	Nitrobenzene	298.2	9.47	8.83	-6.8%	9.09	-4.0%	[50]
N-Heptane	Nitroethane	293.2	19.85	16.93	-14.7%	10.74	-45.9%	[16]
N-Heptane	Nitromethane	298.2	80.04	62.18	-22.3%	70.01	-12.5%	[50]
N-Heptane	N-Methyl-2-Pyrrolidone	298.2	16.77	17.27	3.0%	12.72	-24.2%	[50]
N-Heptane	N-Methyl-2-Pyrrolidone	323.4	16.30	12.29	-24.6%	11.24	-31.0%	[43]
N-Heptane	N-Methyl-2-Pyrrolidone	333.2	14.70	10.96	-25.4%	10.62	-27.8%	[43]
N-Heptane	N-Methyl-2-Pyrrolidone	343.4	13.40	9.82	-26.7%	9.96	-25.7%	[43]
N-Heptane	N-Methylacetamide	303.1	18.51	20.09	8.5%	18.35	-0.9%	[13]
N-Heptane	N-Methylacetamide	318.4	17.05	17.67	3.6%	17.27	1.3%	[13]
N-Heptane	N-Methylacetamide	333.2	16.03	15.52	-3.2%	16.32	1.8%	[13]
N-Heptane	N-Methylformamide	298.2	55.57	59.61	7.3%	M.P.	N.A.	[50]
N-Heptane	N-Methylformamide	303.2	57.72	55.72	-3.5%	M.P.	N.A.	[35]
N-Heptane	N-Methylformamide	313.2	52.46	48.58	-7.4%	M.P.	N.A.	[35]
N-Heptane	N-Methylformamide	323.2	47.54	42.31	-11.0%	M.P.	N.A.	[35]
N-Heptane	N-Methylformamide	333.2	44.04	36.87	-16.3%	M.P.	N.A.	[35]
N-Heptane	N-Nonane	298.2	1.03	0.99	-3.9%	0.99	-3.9%	[50]
N-Heptane	N-Nonane	313.2	0.77	0.99	28.6%	0.99	28.6%	[72]
N-Heptane	N-Nonane	323.2	0.80	0.99	23.8%	0.99	23.8%	[72]
N-Heptane	N-Nonane	333.2	0.84	0.99	17.9%	0.99	17.9%	[72]
N-Heptane	N-Octane	298.2	1.05	1.00	-4.8%	1.00	-4.8%	[50]
N-Heptane	N-Pentane	298.2	1.14	1.01	-11.4%	1.00	-12.3%	[50]
N-Heptane	Phenol	323.2	15.40	16.59	7.7%	15.62	1.4%	[10]
N-Heptane	Phenol	328.2	17.08	15.99	-6.4%	14.84	-13.1%	[14]
N-Heptane	Phenol	343.2	14.83	14.26	-3.8%	12.72	-14.2%	[14]
N-Heptane	Phenol	358.2	13.47	12.66	-6.0%	10.90	-19.1%	[14]
N-Heptane	Phenol	373.2	12.81	11.22	-12.4%	9.35	-27.0%	[14]
N-Heptane	Propionitrile	298.2	13.86	14.85	7.1%	10.62	-23.4%	[50]
N-Heptane	Propionitrile	313.2	13.86	11.72	-15.4%	9.25	-33.2%	125

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N-Heptane	P-Xylene	298.2	1.51	1.48	-2.0%	1.45	-4.0%	[50]
N-Heptane	P-Xylene	313.2	1.41	1.43	1.2%	1.42	0.5%	102
N-Heptane	P-Xylene	313.2	1.22	1.43	17.2%	1.42	16.4%	[72]
N-Heptane	P-Xylene	323.2	1.17	1.40	19.7%	1.40	19.7%	[72]
N-Heptane	P-Xylene	333.2	1.10	1.38	25.5%	1.38	25.5%	[72]
N-Heptane	Pyridine	298.2	8.58	6.97	-18.7%	7.62	-11.1%	588
N-Heptane	Pyridine	298.2	7.43	6.97	-6.2%	7.62	2.6%	[50]
N-Heptane	Pyridine	303.1	8.02	6.60	-17.7%	7.32	-8.7%	588
N-Heptane	Pyridine	313.2	6.67	5.95	-10.8%	6.78	1.6%	588
N-Heptane	Pyridine	313.2	7.18	5.95	-17.2%	6.78	-5.6%	588
N-Heptane	Pyridine	323.2	6.37	5.41	-15.0%	6.30	-1.0%	588
N-Heptane	Pyridine	333.2	5.83	4.94	-15.3%	5.88	0.9%	588
N-Heptane	Pyridine	341.0	4.86	4.63	-4.7%	5.59	15.0%	588
N-Heptane	Pyridine	353.2	4.19	4.20	0.2%	5.15	22.9%	588
N-Heptane	Quinoline	293.2	9.55	9.33	-2.3%	M.G.	N.A.	[37]
N-Heptane	Squalane	298.2	0.70	0.62	-11.4%	0.75	7.1%	[50]
N-Heptane	Sulfolane	303.4	62.02	74.81	20.6%	M.G.	N.A.	[13]
N-Heptane	Sulfolane	317.9	54.00	52.93	-2.0%	M.G.	N.A.	[13]
N-Heptane	Sulfolane	332.6	47.37	38.90	-17.9%	M.G.	N.A.	[13]
N-Heptane	Tetraethylene Glycol DME	303.2	4.79	5.04	5.3%	2.32	-51.5%	[7]
N-Heptane	Tetraethylene Glycol DME	323.2	4.29	4.32	0.8%	2.11	-50.8%	[7]
N-Heptane	Tetraethylene Glycol DME	343.2	3.66	3.79	3.5%	1.94	-47.0%	[7]
N-Heptane	Tetrahydrofuran	298.2	2.29	2.17	-5.2%	1.94	-15.3%	[50]
N-Heptane	Tetrahydrofuran	303.2	1.98	2.12	7.1%	1.89	-4.5%	[15]
N-Heptane	Tetrahydrofuran	313.2	2.02	2.02	0.0%	1.79	-11.4%	[19]
N-Heptane	Tetrahydrofuran	333.2	1.79	1.85	3.4%	1.64	-8.4%	[19]
N-Heptane	Tetrahydrofuran	343.2	1.70	1.79	5.3%	1.57	-7.6%	[15]
N-Heptane	Toluene	298.2	1.76	1.82	3.4%	1.65	-6.3%	[50]
N-Heptane	Tributyl Phosphate	298.6	2.12	2.31	9.0%	M.G.	N.A.	[27]
N-Heptane	Tributyl Phosphate	302.9	2.32	2.25	-3.0%	M.G.	N.A.	[27]
N-Heptane	Tributyl Phosphate	308.6	2.10	2.19	4.3%	M.G.	N.A.	[27]
N-Heptane	Tributyl Phosphate	313.1	2.08	2.13	2.4%	M.G.	N.A.	[27]
N-Heptane	Tributyl Phosphate	323.7	1.92	2.03	5.7%	M.G.	N.A.	[27]
N-Heptane	Tributyl Phosphate	330.0	1.79	1.97	10.1%	M.G.	N.A.	[27]
N-Heptane	Triethylamine	298.2	1.08	1.09	0.9%	1.05	-2.8%	[50]
N-Hexadecane	Acetone	333.2	34.56	18.97	-45.1%	14.07	-59.3%	316
N-Hexadecane	Methyl Ethyl Ketone	333.2	6.38	7.89	23.6%	8.36	30.9%	83
N-Hexadecane	Methyl Ethyl Ketone	353.2	4.67	6.16	31.8%	6.42	37.4%	83
N-Hexane	1,2-Dichloroethane	293.2	5.04	4.84	-4.0%	3.71	-26.4%	[10]
N-Hexane	1,2-Dichloroethane	298.2	5.50	4.63	-15.9%	3.54	-35.7%	119
N-Hexane	1,2-Dichloroethane	298.2	5.17	4.63	-10.4%	3.54	-31.5%	[50]
N-Hexane	1,2-Dichloroethane	318.5	3.99	3.94	-1.3%	2.96	-25.8%	[12]
N-Hexane	1,2-Dichloroethane	337.2	3.59	3.47	-3.3%	2.55	-29.0%	[12]
N-Hexane	1,2-Dichloroethane	354.2	3.01	3.13	4.0%	2.24	-25.6%	[12]
N-Hexane	1,4-Dioxane	298.2	6.70	5.09	-24.0%	5.64	-15.8%	[50]
N-Hexane	1,4-Dioxane	353.2	3.58	3.51	-2.0%	3.70	3.3%	339
N-Hexane	1,5-Dimethyl-2-Pyrrolidinone	298.2	8.98	8.44	-6.0%	M.G.	N.A.	[29]
N-Hexane	1,5-Dimethyl-2-Pyrrolidinone	308.2	8.31	7.61	-8.4%	M.G.	N.A.	[29]
N-Hexane	1,5-Dimethyl-2-Pyrrolidinone	318.2	7.89	6.92	-12.3%	M.G.	N.A.	[29]
N-Hexane	1-Butanol	293.2	5.00	5.21	4.2%	4.84	-3.2%	[10]

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N-Hexane	1-Butanol	298.2	5.12	5.15	0.6%	4.80	-6.3%	[50]
N-Hexane	1-Butanol	308.2	4.83	5.00	3.5%	4.71	-2.5%	[30]
N-Hexane	1-Butanol	318.2	4.66	4.83	3.6%	4.60	-1.3%	[30]
N-Hexane	1-Butanol	328.2	4.67	4.65	-0.4%	4.47	-4.3%	[30]
N-Hexane	1-Butanol	333.2	4.61	4.56	-1.0%	4.40	-4.5%	143
N-Hexane	1-Chlorobutane	293.2	1.73	1.75	1.2%	1.36	-21.4%	[10]
N-Hexane	1-Ethylpyrrolidin-2-One	298.2	8.40	8.42	0.2%	4.34	-48.3%	[29]
N-Hexane	1-Ethylpyrrolidin-2-One	308.2	7.82	7.60	-2.8%	4.16	-46.8%	[29]
N-Hexane	1-Ethylpyrrolidin-2-One	318.2	7.28	6.92	-4.9%	3.99	-45.2%	[29]
N-Hexane	1-Hexanol	293.2	3.16	3.92	24.1%	3.28	3.8%	[28]
N-Hexane	1-Hexanol	313.1	3.05	3.70	21.3%	3.19	4.6%	[28]
N-Hexane	1-Hexanol	313.2	2.91	3.70	27.1%	3.19	9.6%	[28]
N-Hexane	1-Hexanol	322.8	3.02	3.58	18.5%	3.13	3.6%	[28]
N-Hexane	1-Hexanol	332.6	2.85	3.46	21.4%	3.06	7.4%	[28]
N-Hexane	1-Hexanol	333.2	2.69	3.45	28.3%	3.06	13.8%	[28]
N-Hexane	1-Hexanol	333.2	2.45	3.45	40.8%	3.06	24.9%	[81]
N-Hexane	1-Hexene	298.2	1.10	1.01	-8.2%	1.06	-3.6%	[50]
N-Hexane	1-Octanol	293.4	2.70	2.85	5.6%	2.55	-5.6%	[31]
N-Hexane	1-Octanol	298.2	2.67	2.80	4.9%	2.54	-4.9%	[50]
N-Hexane	1-Octanol	298.2	2.81	2.80	-0.4%	2.54	-9.6%	[32]
N-Hexane	1-Octanol	303.5	2.62	2.74	4.6%	2.53	-3.4%	[31]
N-Hexane	1-Octanol	313.6	2.66	2.63	-1.1%	2.49	-6.4%	[31]
N-Hexane	1-Octanol	323.4	2.53	2.53	0.0%	2.45	-3.2%	[31]
N-Hexane	1-Octene	298.2	1.02	1.01	-1.0%	1.06	3.9%	[50]
N-Hexane	1-Pentanol	303.5	4.11	4.19	1.9%	3.83	-6.8%	[33]
N-Hexane	1-Pentanol	308.2	4.26	4.13	-3.1%	3.80	-10.8%	[30]
N-Hexane	1-Pentanol	313.2	4.10	4.07	-0.7%	3.76	-8.3%	[33]
N-Hexane	1-Pentanol	318.2	4.17	4.00	-4.1%	3.72	-10.8%	[30]
N-Hexane	1-Pentanol	323.5	3.96	3.93	-0.8%	3.68	-7.1%	[33]
N-Hexane	1-Pentanol	328.2	3.68	3.86	4.9%	3.64	-1.1%	[30]
N-Hexane	1-Phenyl-1-Butanone	298.1	3.69	3.88	5.1%	3.72	0.8%	[34]
N-Hexane	1-Propanol	298.2	6.73	6.65	-1.2%	6.49	-3.6%	[50]
N-Hexane	1-Propanol	308.2	6.45	6.47	0.3%	6.33	-1.9%	[47]
N-Hexane	2,2,4-Trimethylpentane	298.2	1.02	1.01	-1.0%	1.00	-2.0%	[50]
N-Hexane	2-Heptanone	298.2	2.21	2.18	-1.4%	2.45	10.9%	[50]
N-Hexane	2-Methyl-2-Propanol	303.3	3.81	4.40	15.5%	3.03	-20.5%	[28]
N-Hexane	2-Methyl-2-Propanol	313.1	3.55	4.22	18.9%	2.97	-16.3%	[28]
N-Hexane	2-Methyl-2-Propanol	313.2	3.64	4.22	15.8%	2.97	-18.5%	2
N-Hexane	2-Methyl-2-Propanol	322.8	3.31	4.05	22.4%	2.90	-12.4%	[28]
N-Hexane	2-Nitropropane	293.2	7.50	7.40	-1.3%	5.57	-25.7%	[10]
N-Hexane	2-Pentanone	298.2	3.01	3.12	3.7%	3.42	13.6%	[50]
N-Hexane	2-Pyrrolidone	303.2	42.56	47.31	11.2%	M.G.	N.A.	[35]
N-Hexane	2-Pyrrolidone	313.2	38.81	39.28	1.2%	M.G.	N.A.	[35]
N-Hexane	2-Pyrrolidone	323.2	35.60	32.99	-7.3%	M.G.	N.A.	[35]
N-Hexane	2-Pyrrolidone	333.2	33.11	28.02	-15.4%	M.G.	N.A.	[35]
N-Hexane	Acetic Acid	298.2	16.26	15.60	-4.1%	10.70	-34.2%	[50]
N-Hexane	Acetone	253.2	13.09	11.34	-13.4%	9.37	-28.4%	217
N-Hexane	Acetone	268.2	11.66	9.09	-22.0%	8.05	-30.9%	217
N-Hexane	Acetone	293.2	7.94	6.70	-15.6%	6.38	-19.7%	217
N-Hexane	Acetone	298.2	7.15	6.36	-11.0%	6.11	-14.5%	[50]
N-Hexane	Acetone	298.2	6.50	6.36	-2.2%	6.11	-6.0%	[62]
N-Hexane	Acetone	300.9	6.41	6.19	-3.4%	5.97	-6.9%	[17]

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N-Hexane	Acetone	303.2	6.78	6.05	-10.8%	5.85	-13.7%	[18]
N-Hexane	Acetone	303.2	6.51	6.05	-7.1%	5.85	-10.1%	[18]
N-Hexane	Acetone	306.9	6.24	5.83	-6.6%	5.67	-9.1%	[17]
N-Hexane	Acetone	308.2	6.50	5.76	-11.4%	5.61	-13.7%	[75]
N-Hexane	Acetone	313.3	5.68	5.49	-3.3%	5.38	-5.3%	[18]
N-Hexane	Acetone	316.7	5.54	5.33	-3.8%	5.24	-5.4%	[17]
N-Hexane	Acetone	318.2	5.98	5.26	-12.1%	5.17	-13.6%	217
N-Hexane	Acetone	324.4	5.24	4.99	-4.8%	4.93	-5.9%	[17]
N-Hexane	Acetone	328.4	4.95	4.83	-2.4%	4.78	-3.4%	[17]
N-Hexane	Acetone	329.4	5.39	4.79	-11.1%	4.74	-12.1%	[11]
N-Hexane	Acetone	333.2	5.10	4.65	-8.8%	4.61	-9.6%	[62]
N-Hexane	Acetone	373.2	4.50	3.56	-20.9%	3.50	-22.2%	[62]
N-Hexane	Acetonitrile	298.2	24.00	27.77	15.7%	26.03	8.5%	[36]
N-Hexane	Acetonitrile	298.2	27.97	27.77	-0.7%	26.03	-6.9%	[50]
N-Hexane	Acetonitrile	298.2	25.50	27.77	8.9%	26.03	2.1%	[62]
N-Hexane	Acetonitrile	333.2	15.80	14.49	-8.3%	14.45	-8.5%	[62]
N-Hexane	Acetonitrile	373.2	10.80	8.34	-22.8%	8.31	-23.1%	[62]
N-Hexane	Acetophenone	293.2	6.84	6.32	-7.6%	9.76	42.7%	[10]
N-Hexane	Acetophenone	298.2	6.39	6.01	-5.9%	9.37	46.6%	[50]
N-Hexane	Acetophenone	298.2	6.74	6.01	-10.8%	9.37	39.0%	[65]
N-Hexane	Aniline	293.2	24.87	22.43	-9.8%	22.01	-11.5%	[37]
N-Hexane	Aniline	293.2	25.70	22.43	-12.7%	22.01	-14.4%	[10]
N-Hexane	Aniline	298.2	27.00	20.77	-23.1%	20.89	-22.6%	[62]
N-Hexane	Aniline	298.2	27.09	20.77	-23.3%	20.89	-22.9%	[66]
N-Hexane	Aniline	298.2	26.25	20.77	-20.9%	20.89	-20.4%	[66]
N-Hexane	Aniline	298.2	26.63	20.77	-22.0%	20.89	-21.6%	[65]
N-Hexane	Aniline	323.2	14.00	14.68	4.9%	15.66	11.9%	[62]
N-Hexane	Aniline	373.2	8.00	8.52	6.5%	7.55	-5.6%	[62]
N-Hexane	Anisole	293.2	3.94	3.87	-1.8%	2.86	-27.4%	[10]
N-Hexane	Anisole	298.2	3.79	3.73	-1.6%	2.79	-26.4%	[50]
N-Hexane	Anisole	333.2	2.90	3.00	3.5%	2.36	-18.6%	54
N-Hexane	Anisole	343.2	2.63	2.85	8.3%	2.26	-14.1%	54
N-Hexane	Benzene	293.2	2.23	2.20	-1.3%	2.21	-0.9%	[58]
N-Hexane	Benzene	293.2	2.21	2.20	-0.5%	2.21	0.0%	[10]
N-Hexane	Benzene	298.2	2.11	2.15	1.9%	2.16	2.4%	[50]
N-Hexane	Benzene	313.2	2.01	2.01	0.1%	2.01	0.1%	105
N-Hexane	Benzene	353.3	1.58	1.76	11.4%	1.71	8.2%	[11]
N-Hexane	Benzonitrile	293.2	6.68	6.87	2.8%	M.G.	N.A.	[10]
N-Hexane	Benzonitrile	298.2	6.25	6.52	4.3%	M.G.	N.A.	[50]
N-Hexane	Benzyl Acetate	298.2	5.28	5.03	-4.7%	4.11	-22.2%	[10]
N-Hexane	Benzyl Alcohol	298.2	12.82	12.65	-1.3%	10.00	-22.0%	[50]
N-Hexane	Benzyl Alcohol	298.2	13.46	12.65	-6.0%	10.00	-25.7%	[67]
N-Hexane	Butanal	308.2	2.79	3.18	14.0%	2.85	2.2%	[38]
N-Hexane	Butanal	328.2	2.67	2.85	6.7%	2.74	2.5%	[38]
N-Hexane	Butanal	347.2	2.50	2.60	4.0%	2.63	5.3%	[38]
N-Hexane	Butyl Acetate	298.2	2.17	2.17	0.0%	2.84	30.9%	[50]
N-Hexane	Butyl Ether	293.2	0.99	1.14	15.2%	1.08	9.1%	[5]
N-Hexane	Butyl Ether	308.2	1.07	1.13	6.1%	1.07	0.5%	136
N-Hexane	Butyronitrile	298.2	6.48	6.45	-0.5%	5.42	-16.4%	[50]
N-Hexane	Carbon Disulfide	298.2	2.38	2.51	5.5%	2.65	11.3%	[50]
N-Hexane	Carbon Tetrachloride	293.2	1.33	1.38	3.8%	1.35	1.5%	[10]
N-Hexane	Carbon Tetrachloride	298.2	1.35	1.36	0.7%	1.33	-1.5%	[50]

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N-Hexane	Carbon Tetrachloride	313.2	1.28	1.33	4.2%	1.29	1.1%	95
N-Hexane	Chlorobenzene	298.2	2.22	2.21	-0.5%	2.70	21.6%	[50]
N-Hexane	Chloroform	298.2	2.03	2.12	4.4%	1.99	-2.0%	[50]
N-Hexane	Chloroform	308.2	2.08	2.03	-2.5%	1.90	-8.8%	265
N-Hexane	Chloroform	318.2	1.98	1.94	-1.9%	1.82	-8.0%	265
N-Hexane	Chloroform	319.8	1.79	1.93	7.8%	1.81	1.1%	[12]
N-Hexane	Chloroform	328.2	1.73	1.87	8.0%	1.75	1.1%	265
N-Hexane	Chloroform	331.9	1.66	1.84	10.8%	1.73	4.2%	[12]
N-Hexane	Chloroform	334.3	1.64	1.83	11.6%	1.71	4.3%	[11]
N-Hexane	Chloroform	334.3	1.55	1.83	18.1%	1.71	10.3%	[11]
N-Hexane	Cyclohexane	298.2	1.18	1.18	0.0%	1.09	-7.6%	[50]
N-Hexane	Cyclohexane	323.7	1.09	1.16	6.4%	1.07	-1.8%	[17]
N-Hexane	Cyclohexane	332.9	1.08	1.15	6.5%	1.06	-1.9%	[17]
N-Hexane	Cyclohexane	353.3	1.05	1.14	8.6%	1.04	-1.0%	[17]
N-Hexane	Cyclohexanone	293.2	4.46	4.32	-3.1%	3.15	-29.4%	[10]
N-Hexane	Cyclohexanone	298.2	4.30	4.16	-3.3%	3.08	-28.4%	[50]
N-Hexane	Dichloromethane	298.2	3.14	3.38	7.8%	2.79	-11.0%	331
N-Hexane	Dichloromethane	298.2	3.42	3.38	-1.2%	2.79	-18.4%	[50]
N-Hexane	Diethyl Phthalate	303.2	4.84	4.98	2.9%	M.G.	N.A.	[39]
N-Hexane	Diethyl Phthalate	313.2	4.53	4.58	1.1%	M.G.	N.A.	[39]
N-Hexane	Diethyl Phthalate	323.2	4.32	4.24	-1.9%	M.G.	N.A.	[39]
N-Hexane	Diethyl Phthalate	333.2	4.09	3.95	-3.4%	M.G.	N.A.	[39]
N-Hexane	Dimethyl Sulfoxide	283.2	96.00	104.50	8.9%	106.24	10.7%	[40]
N-Hexane	Dimethyl Sulfoxide	298.2	68.68	68.32	-0.5%	77.16	12.3%	[50]
N-Hexane	Dimethyl Sulfoxide	298.2	75.00	68.32	-8.9%	77.16	2.9%	[62]
N-Hexane	Dimethyl Sulfoxide	313.2	72.00	47.26	-34.4%	57.32	-20.4%	[68]
N-Hexane	Dimethyl Sulfoxide	333.2	39.00	31.04	-20.4%	39.84	2.2%	[62]
N-Hexane	Dimethyl Sulfoxide	373.2	22.00	16.10	-26.8%	21.22	-3.5%	[62]
N-Hexane	Epsilon-Caprolactone	303.2	12.90	13.55	5.0%	M.G.	N.A.	[41]
N-Hexane	Epsilon-Caprolactone	318.2	11.90	11.12	-6.6%	M.G.	N.A.	[41]
N-Hexane	Epsilon-Caprolactone	333.2	10.80	9.36	-13.3%	M.G.	N.A.	[41]
N-Hexane	Ethanol	293.2	9.57	12.11	26.5%	10.47	9.4%	[28]
N-Hexane	Ethanol	293.2	12.00	12.11	0.9%	10.47	-12.8%	[10]
N-Hexane	Ethanol	298.2	10.59	11.93	12.7%	10.31	-2.6%	[50]
N-Hexane	Ethanol	298.2	12.00	11.93	-0.6%	10.31	-14.1%	[62]
N-Hexane	Ethanol	303.2	12.70	11.72	-7.7%	10.13	-20.2%	[18]
N-Hexane	Ethanol	313.2	8.21	11.22	36.7%	9.73	18.5%	[28]
N-Hexane	Ethanol	313.2	11.60	11.22	-3.3%	9.73	-16.1%	[18]
N-Hexane	Ethanol	313.2	9.90	11.22	13.3%	9.73	-1.7%	[75]
N-Hexane	Ethanol	322.2	10.00	10.71	7.1%	9.32	-6.8%	[48]
N-Hexane	Ethanol	333.2	7.24	10.04	38.7%	8.76	21.0%	[28]
N-Hexane	Ethanol	333.2	9.70	10.04	3.5%	8.76	-9.7%	[62]
N-Hexane	Ethanol	350.9	8.10	8.94	10.4%	7.76	-4.2%	[12]
N-Hexane	Ethanol	354.2	8.70	8.74	0.5%	7.56	-13.1%	[48]
N-Hexane	Ethanol	373.2	8.40	7.63	-9.2%	6.41	-23.7%	[62]
N-Hexane	Ethyl Acetate	293.2	3.49	3.41	-2.3%	3.42	-2.0%	[10]
N-Hexane	Ethyl Acetate	298.2	3.60	3.30	-8.3%	3.30	-8.3%	[50]
N-Hexane	Ethyl Acetate	303.2	3.33	3.20	-3.9%	3.18	-4.5%	[75]
N-Hexane	Ethyl Acetate	308.2	3.09	3.10	0.3%	3.07	-0.6%	[12]
N-Hexane	Ethyl Acetate	324.4	2.77	2.84	2.5%	2.76	-0.4%	[12]
N-Hexane	Ethyl Acetate	348.4	2.41	2.54	5.4%	2.40	-0.4%	[12]
N-Hexane	Ethyl Benzoate	313.2	2.99	2.94	-1.7%	M.G.	N.A.	[41]

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N-Hexane	Ethyl Benzoate	323.2	2.89	2.80	-3.1%	M.G.	N.A.	[41]
N-Hexane	Ethyl Benzoate	333.2	2.81	2.67	-5.0%	M.G.	N.A.	[41]
N-Hexane	Ethyl Benzoate	343.2	2.73	2.55	-6.6%	M.G.	N.A.	[41]
N-Hexane	Isopropanol	298.2	6.53	6.19	-5.2%	5.18	-20.7%	[50]
N-Hexane	Isopropanol	308.2	7.40	6.01	-18.8%	5.06	-31.6%	[47]
N-Hexane	Isopropanol	323.9	5.68	5.66	-0.4%	4.82	-15.1%	[17]
N-Hexane	Isopropanol	328.2	5.84	5.55	-4.9%	4.74	-18.8%	224
N-Hexane	Isopropanol	332.7	5.48	5.44	-0.7%	4.66	-15.0%	[17]
N-Hexane	Isopropanol	343.8	5.23	5.17	-1.1%	4.43	-15.3%	[17]
N-Hexane	Isopropanol	354.6	5.11	4.90	-4.1%	4.19	-18.0%	[17]
N-Hexane	Methanol	298.2	25.89	29.09	12.4%	22.81	-11.9%	[50]
N-Hexane	Methanol	298.2	27.00	29.09	7.7%	22.81	-15.5%	[62]
N-Hexane	Methanol	303.2	25.90	28.29	9.2%	22.20	-14.3%	[18]
N-Hexane	Methanol	313.2	23.50	26.44	12.5%	21.04	-10.5%	[18]
N-Hexane	Methanol	333.2	19.00	22.31	17.4%	18.94	-0.3%	[62]
N-Hexane	Methanol	373.2	13.50	14.75	9.3%	15.25	13.0%	[62]
N-Hexane	Methyl Acetate	298.2	5.86	5.40	-7.8%	5.01	-14.5%	[50]
N-Hexane	Methyl Ethyl Ketone	298.2	4.09	4.07	-0.5%	4.36	6.6%	[50]
N-Hexane	Methyl Ethyl Ketone	298.2	4.00	4.07	1.8%	4.36	9.0%	[18]
N-Hexane	Methyl Ethyl Ketone	298.2	4.30	4.07	-5.3%	4.36	1.4%	[10]
N-Hexane	Methyl Ethyl Ketone	303.2	4.27	3.93	-8.0%	4.22	-1.2%	[18]
N-Hexane	Methyl Ethyl Ketone	313.1	3.98	3.67	-7.8%	3.97	-0.3%	[18]
N-Hexane	Methyl Ethyl Ketone	313.2	4.12	3.67	-10.9%	3.97	-3.6%	[18]
N-Hexane	Methyl Ethyl Ketone	323.2	3.82	3.44	-9.9%	3.74	-2.1%	[18]
N-Hexane	Methyl Ethyl Ketone	333.2	3.65	3.25	-11.0%	3.53	-3.3%	[18]
N-Hexane	Methyl Ethyl Ketone	333.2	3.15	3.25	3.2%	3.53	12.1%	[62]
N-Hexane	Methyl Ethyl Ketone	373.2	2.60	2.67	2.7%	2.86	10.0%	[62]
N-Hexane	Methyl Isobutyl Ketone	293.2	2.26	2.62	15.9%	2.90	28.3%	[5]
N-Hexane	Methyl Isobutyl Ketone	328.2	2.50	2.24	-10.4%	2.52	0.8%	[49]
N-Hexane	Methyl Isobutyl Ketone	348.2	2.25	2.08	-7.6%	2.35	4.4%	[49]
N-Hexane	Methyl Isobutyl Ketone	388.2	1.85	1.85	0.0%	2.07	11.9%	[49]
N-Hexane	Methyl Tert-Butyl Ether	303.2	1.16	1.35	16.4%	1.26	8.6%	[56]
N-Hexane	Methyl Tert-Butyl Ether	323.2	1.15	1.31	13.9%	1.22	6.1%	[56]
N-Hexane	N,N-Dibutylformamide	302.8	2.75	3.14	14.1%	2.83	2.9%	[13]
N-Hexane	N,N-Dibutylformamide	318.3	2.58	2.86	10.8%	2.74	6.2%	[13]
N-Hexane	N,N-Dibutylformamide	332.4	2.45	2.66	8.7%	2.66	8.7%	[13]
N-Hexane	N,N-Diethylacetamide	303.2	5.02	5.13	2.2%	2.31	-54.0%	[39]
N-Hexane	N,N-Diethylacetamide	313.2	4.70	4.74	0.9%	2.23	-52.6%	[39]
N-Hexane	N,N-Diethylacetamide	323.2	4.45	4.40	-1.1%	2.15	-51.7%	[39]
N-Hexane	N,N-Diethylacetamide	333.2	4.21	4.10	-2.6%	2.09	-50.4%	[39]
N-Hexane	N,N-Dimethylacetamide	303.2	9.77	9.79	0.2%	8.21	-15.9%	[13]
N-Hexane	N,N-Dimethylacetamide	317.6	8.23	8.29	0.8%	7.25	-11.9%	[13]
N-Hexane	N,N-Dimethylacetamide	333.3	6.94	7.08	2.1%	6.43	-7.3%	[13]
N-Hexane	N,N-Dimethylformamide	283.2	23.70	20.91	-11.8%	18.88	-20.3%	[40]
N-Hexane	N,N-Dimethylformamide	293.2	20.80	17.65	-15.1%	16.73	-19.6%	[10]
N-Hexane	N,N-Dimethylformamide	298.2	17.00	16.30	-4.1%	15.79	-7.1%	[62]
N-Hexane	N,N-Dimethylformamide	298.2	17.90	16.30	-8.9%	15.79	-11.8%	[65]
N-Hexane	N,N-Dimethylformamide	333.2	11.50	10.15	-11.7%	10.96	-4.7%	[62]
N-Hexane	N,N-Dimethylformamide	373.2	8.00	6.75	-15.6%	7.74	-3.3%	[62]
N-Hexane	N-Decane	298.2	0.99	0.97	-2.0%	0.98	-1.0%	[50]
N-Hexane	N-Decane	333.2	0.97	0.97	0.0%	0.98	1.0%	[81]
N-Hexane	N-Decane	343.2	0.96	0.97	1.0%	0.98	2.1%	[81]

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N-Hexane	N-Dodecane	298.2	1.00	0.95	-5.0%	0.95	-5.0%	[50]
N-Hexane	N-Ethylacetamide	303.2	9.23	9.93	7.6%	M.G.	N.A.	[39]
N-Hexane	N-Ethylacetamide	313.2	8.95	9.31	4.0%	M.G.	N.A.	[39]
N-Hexane	N-Ethylacetamide	323.2	8.79	8.71	-0.9%	M.G.	N.A.	[39]
N-Hexane	N-Ethylacetamide	333.2	8.51	8.15	-4.2%	M.G.	N.A.	[39]
N-Hexane	N-Formylmorpholine	313.3	32.10	29.15	-9.2%	M.G.	N.A.	[43]
N-Hexane	N-Formylmorpholine	332.7	24.60	21.46	-12.8%	M.G.	N.A.	[43]
N-Hexane	N-Formylmorpholine	352.5	20.60	16.35	-20.6%	M.G.	N.A.	[43]
N-Hexane	N-Formylmorpholine	373.4	17.00	12.74	-25.1%	M.G.	N.A.	[43]
N-Hexane	N-Heptane	293.2	1.00	1.00	0.0%	1.00	0.0%	[10]
N-Hexane	N-Heptane	298.2	1.04	1.00	-3.8%	1.00	-3.8%	[50]
N-Hexane	N-Heptane	298.2	1.00	1.00	0.0%	1.00	0.0%	[62]
N-Hexane	N-Heptane	333.2	1.00	1.00	0.0%	1.00	0.0%	[62]
N-Hexane	N-Heptane	373.2	1.00	1.00	0.0%	1.00	0.0%	[62]
N-Hexane	N-Hexadecane	293.2	0.91	0.87	-4.4%	0.90	-1.1%	[70]
N-Hexane	N-Hexadecane	293.2	0.90	0.87	-3.3%	0.90	0.0%	[77]
N-Hexane	N-Hexadecane	298.2	0.90	0.87	-3.3%	0.90	0.0%	[70]
N-Hexane	N-Hexadecane	298.2	0.90	0.87	-3.3%	0.90	0.0%	[50]
N-Hexane	N-Hexadecane	298.2	0.90	0.87	-3.1%	0.90	0.2%	[6]
N-Hexane	N-Hexadecane	298.2	0.90	0.87	-3.3%	0.90	0.0%	[65]
N-Hexane	N-Hexadecane	303.2	0.90	0.87	-3.3%	0.90	0.0%	[70]
N-Hexane	N-Hexadecane	308.2	0.90	0.86	-4.4%	0.90	0.0%	[84]
N-Hexane	N-Hexadecane	313.2	0.90	0.86	-4.4%	0.90	0.0%	[70]
N-Hexane	N-Hexadecane	323.2	0.90	0.86	-4.4%	0.90	0.0%	[70]
N-Hexane	N-Hexadecane	333.2	0.91	0.86	-5.5%	0.90	-1.1%	[70]
N-Hexane	N-Hexadecane	333.2	0.90	0.86	-4.4%	0.90	0.0%	[71]
N-Hexane	N-Hexadecane	393.2	0.88	0.85	-3.4%	0.90	2.3%	[71]
N-Hexane	N-Hexadecane	453.2	0.86	0.84	-2.3%	0.90	4.7%	[71]
N-Hexane	N-Hexane	298.2	1.02	1.00	-2.0%	1.00	-2.0%	[50]
N-Hexane	Nitrobenzene	293.2	8.20	7.87	-4.0%	8.12	-1.0%	[10]
N-Hexane	Nitrobenzene	298.2	8.17	7.44	-8.9%	7.85	-3.9%	[50]
N-Hexane	Nitrobenzene	298.2	7.00	7.44	6.3%	7.85	12.1%	[62]
N-Hexane	Nitrobenzene	298.2	8.24	7.44	-9.7%	7.85	-4.7%	[65]
N-Hexane	Nitrobenzene	333.2	5.10	5.34	4.7%	6.17	21.0%	[62]
N-Hexane	Nitrobenzene	373.2	3.70	4.03	8.9%	4.57	23.5%	[62]
N-Hexane	Nitroethane	293.2	11.40	13.17	15.5%	8.88	-22.1%	[10]
N-Hexane	Nitromethane	293.2	58.00	47.26	-18.5%	53.21	-8.3%	[10]
N-Hexane	Nitromethane	298.2	50.32	41.62	-17.3%	48.83	-3.0%	[50]
N-Hexane	Nitromethane	298.2	48.00	41.62	-13.3%	48.83	1.7%	[62]
N-Hexane	Nitromethane	333.2	22.00	19.76	-10.2%	29.09	32.2%	[62]
N-Hexane	Nitromethane	373.2	12.00	10.62	-11.5%	18.98	58.2%	[62]
N-Hexane	N-Methyl-2-Pyrrolidone	298.2	13.13	14.33	9.1%	10.26	-21.9%	[50]
N-Hexane	N-Methyl-2-Pyrrolidone	323.4	13.50	10.51	-22.1%	9.21	-31.8%	[43]
N-Hexane	N-Methyl-2-Pyrrolidone	333.2	12.70	9.47	-25.4%	8.76	-31.0%	[43]
N-Hexane	N-Methyl-2-Pyrrolidone	343.4	11.60	8.57	-26.1%	8.28	-28.6%	[43]
N-Hexane	N-Methylacetamide	303.0	15.24	16.03	5.2%	15.04	-1.3%	[13]
N-Hexane	N-Methylacetamide	318.4	13.89	14.26	2.7%	14.25	2.6%	[13]
N-Hexane	N-Methylacetamide	333.8	12.73	12.62	-0.9%	13.54	6.4%	[13]
N-Hexane	N-Methylformamide	298.2	37.14	42.46	14.3%	M.P.	N.A.	[50]
N-Hexane	N-Methylformamide	303.2	41.39	39.97	-3.4%	M.P.	N.A.	[35]
N-Hexane	N-Methylformamide	313.2	38.46	35.34	-8.1%	M.P.	N.A.	[35]
N-Hexane	N-Methylformamide	323.2	36.06	31.22	-13.4%	M.P.	N.A.	[35]

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N-Hexane	N-Methylformamide	333.2	33.94	27.60	-18.7%	M.P.	N.A.	[35]
N-Hexane	N-Nonane	298.2	1.01	0.99	-2.0%	0.99	-2.0%	[50]
N-Hexane	N-Nonane	313.2	0.76	0.98	28.9%	0.99	30.3%	[72]
N-Hexane	N-Nonane	323.2	0.80	0.98	22.5%	0.99	23.8%	[72]
N-Hexane	N-Nonane	333.2	0.98	0.98	0.0%	0.99	1.0%	[81]
N-Hexane	N-Nonane	333.2	0.85	0.98	15.3%	0.99	16.5%	[72]
N-Hexane	N-Octane	298.2	1.03	0.99	-3.9%	0.99	-3.9%	[50]
N-Hexane	N-Octane	333.2	0.99	0.99	0.0%	0.99	0.0%	[81]
N-Hexane	N-Pentane	298.2	1.12	1.01	-9.8%	1.00	-10.7%	[50]
N-Hexane	Phenol	298.2	17.50	15.62	-10.7%	15.56	-11.1%	[62]
N-Hexane	Phenol	323.2	13.00	13.45	3.5%	12.46	-4.2%	[10]
N-Hexane	Phenol	328.2	14.37	13.01	-9.5%	11.91	-17.1%	[14]
N-Hexane	Phenol	333.2	12.00	12.57	4.8%	11.39	-5.1%	[62]
N-Hexane	Phenol	343.2	12.85	11.72	-8.8%	10.41	-19.0%	[14]
N-Hexane	Phenol	358.2	12.10	10.52	-13.1%	9.10	-24.8%	[14]
N-Hexane	Phenol	373.2	8.70	9.43	8.4%	7.95	-8.6%	[62]
N-Hexane	Phenol	373.2	11.70	9.43	-19.4%	7.95	-32.1%	[14]
N-Hexane	Propionitrile	293.2	11.00	12.78	16.2%	9.65	-12.3%	[10]
N-Hexane	Propionitrile	298.2	10.94	11.83	8.1%	9.25	-15.4%	[50]
N-Hexane	Propionitrile	298.2	10.20	11.83	16.0%	9.25	-9.3%	[62]
N-Hexane	Propionitrile	313.2	13.80	9.58	-30.6%	8.19	-40.7%	126
N-Hexane	Propionitrile	333.2	7.40	7.54	1.9%	7.03	-5.0%	[62]
N-Hexane	Propionitrile	373.2	5.50	5.17	-6.0%	5.34	-2.9%	[62]
N-Hexane	P-Xylene	293.2	1.44	1.50	4.2%	1.53	6.3%	[10]
N-Hexane	P-Xylene	298.2	1.51	1.48	-2.0%	1.52	0.7%	[50]
N-Hexane	P-Xylene	313.2	1.47	1.44	-2.1%	1.49	1.3%	103
N-Hexane	P-Xylene	313.2	1.25	1.44	15.2%	1.49	19.2%	[72]
N-Hexane	P-Xylene	323.2	1.20	1.41	17.5%	1.48	23.3%	[72]
N-Hexane	P-Xylene	333.2	1.14	1.39	21.9%	1.46	28.1%	[72]
N-Hexane	Pyridine	298.2	7.87	6.22	-21.0%	7.30	-7.3%	59
N-Hexane	Pyridine	298.2	6.52	6.22	-4.6%	7.30	12.0%	[50]
N-Hexane	Pyridine	298.2	6.20	6.22	0.3%	7.30	17.7%	[62]
N-Hexane	Pyridine	303.2	7.48	5.93	-20.7%	7.04	-5.9%	59
N-Hexane	Pyridine	313.2	6.77	5.40	-20.3%	6.58	-2.9%	59
N-Hexane	Pyridine	323.2	6.22	4.95	-20.4%	6.18	-0.6%	59
N-Hexane	Pyridine	328.2	5.96	4.74	-20.5%	5.99	0.4%	59
N-Hexane	Pyridine	333.2	4.80	4.56	-5.0%	5.82	21.3%	[62]
N-Hexane	Pyridine	373.2	3.80	3.46	-8.9%	4.57	20.3%	[62]
N-Hexane	Quinoline	293.2	8.51	7.91	-7.1%	M.G.	N.A.	[37]
N-Hexane	Quinoline	298.2	6.50	7.52	15.7%	M.G.	N.A.	[10]
N-Hexane	Squalane	298.2	0.65	0.56	-13.8%	0.72	10.8%	[50]
N-Hexane	Sulfolane	303.8	46.99	50.72	7.9%	M.G.	N.A.	[13]
N-Hexane	Sulfolane	317.9	41.08	37.53	-8.6%	M.G.	N.A.	[13]
N-Hexane	Sulfolane	332.8	35.98	28.34	-21.2%	M.G.	N.A.	[13]
N-Hexane	Tetraethylene Glycol DME	303.2	4.05	4.18	3.3%	2.04	-49.6%	[7]
N-Hexane	Tetraethylene Glycol DME	323.2	3.59	3.64	1.3%	1.88	-47.7%	[7]
N-Hexane	Tetraethylene Glycol DME	343.2	3.20	3.24	1.4%	1.75	-45.2%	[7]
N-Hexane	Tetrahydrofuran	298.2	2.19	2.15	-1.8%	1.93	-11.9%	[50]
N-Hexane	Tetrahydrofuran	313.2	1.95	2.01	3.1%	1.80	-7.7%	[19]
N-Hexane	Tetrahydrofuran	333.2	1.82	1.86	2.2%	1.66	-8.8%	[19]
N-Hexane	Toluene	293.2	1.80	1.88	4.4%	1.74	-3.3%	[33]
N-Hexane	Toluene	293.2	1.87	1.88	0.5%	1.74	-7.0%	[33]

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N-Hexane	Toluene	293.2	2.10	1.88	-10.5%	1.74	-17.1%	[30]
N-Hexane	Toluene	293.2	1.74	1.88	8.0%	1.74	0.0%	[10]
N-Hexane	Toluene	298.2	1.74	1.84	5.7%	1.72	-1.1%	[50]
N-Hexane	Toluene	303.2	1.77	1.81	2.3%	1.70	-4.0%	[33]
N-Hexane	Toluene	303.2	1.85	1.81	-2.2%	1.70	-8.1%	[30]
N-Hexane	Toluene	313.2	1.93	1.75	-9.3%	1.66	-14.0%	[33]
N-Hexane	Toluene	313.2	1.62	1.75	8.0%	1.66	2.5%	[30]
N-Hexane	Tributyl Phosphate	298.6	1.92	1.93	0.5%	M.G.	N.A.	[27]
N-Hexane	Tributyl Phosphate	302.9	1.99	1.89	-5.0%	M.G.	N.A.	[27]
N-Hexane	Tributyl Phosphate	308.6	1.88	1.84	-2.1%	M.G.	N.A.	[27]
N-Hexane	Tributyl Phosphate	313.1	1.80	1.80	0.0%	M.G.	N.A.	[27]
N-Hexane	Tributyl Phosphate	323.7	1.72	1.72	0.0%	M.G.	N.A.	[27]
N-Hexane	Tributyl Phosphate	330.0	1.65	1.67	1.2%	M.G.	N.A.	[27]
N-Hexane	Triethylamine	298.2	1.07	1.06	-0.9%	1.04	-2.8%	[50]
N-Hexane	Triethylamine	323.5	1.06	1.05	-0.9%	1.03	-2.8%	[12]
N-Hexane	Triethylamine	348.7	1.06	1.05	-0.9%	1.02	-3.8%	[12]
N-Hexane	Triethylamine	359.3	1.06	1.05	-0.9%	1.02	-3.8%	[12]
Nitroethane	1,2-Dichloroethane	318.5	1.49	1.23	-17.4%	0.65	-56.4%	[12]
Nitroethane	1,2-Dichloroethane	337.2	1.41	1.21	-14.2%	0.62	-56.0%	[12]
Nitroethane	1,2-Dichloroethane	354.2	1.39	1.20	-13.7%	0.58	-58.3%	[12]
Nitroethane	1-Octanol	298.2	7.45	7.36	-1.2%	4.39	-41.1%	[3]
Nitroethane	2,2,4-Trimethylpentane	293.2	18.90	19.32	2.2%	7.62	-59.7%	[10]
Nitroethane	N-Heptane	293.2	19.80	19.96	0.8%	8.22	-58.5%	[10]
Nitroethane	N-Hexadecane	298.2	14.44	14.82	2.6%	4.92	-65.9%	[6]
Nitroethane	N-Hexane	298.1	20.70	18.60	-10.1%	8.42	-59.3%	[12]
Nitroethane	N-Hexane	316.1	13.20	13.65	3.4%	6.98	-47.1%	[12]
Nitroethane	N-Hexane	332.0	12.30	10.79	-12.3%	6.30	-48.8%	[12]
Nitroethane	N-Hexane	339.4	10.00	9.78	-2.2%	6.11	-38.9%	[12]
Nitroethane	N-Octane	293.2	19.10	19.48	2.0%	7.63	-60.1%	[10]
Nitroethane	Toluene	342.7	2.35	2.38	1.3%	1.80	-23.4%	[12]
Nitroethane	Toluene	381.0	2.10	2.05	-2.4%	1.69	-19.5%	[12]
Nitromethane	1,1-Dichloroethane	298.2	1.72	2.13	23.8%	2.70	57.0%	[16]
Nitromethane	1,2-Dichloroethane	318.5	1.86	1.91	2.7%	1.00	-46.2%	[12]
Nitromethane	1,2-Dichloroethane	343.9	1.73	1.77	2.3%	0.91	-47.4%	[12]
Nitromethane	1,2-Dichloroethane	355.3	1.63	1.72	5.5%	0.87	-46.6%	[12]
Nitromethane	1,4-Dioxane	298.2	1.16	1.33	14.7%	1.16	0.0%	[16]
Nitromethane	1-Butanol	293.2	9.10	8.86	-2.6%	8.93	-1.9%	[10]
Nitromethane	1-Chlorobutane	293.2	5.40	6.81	26.1%	4.44	-17.8%	[10]
Nitromethane	1-Octanol	293.2	10.40	10.95	5.3%	8.61	-17.2%	[10]
Nitromethane	1-Octanol	298.2	9.79	10.19	4.1%	7.80	-20.3%	[3]
Nitromethane	1-Octanol	298.2	8.58	10.19	18.8%	7.80	-9.1%	[69]
Nitromethane	1-Octanol	298.2	9.61	10.19	6.0%	7.80	-18.8%	[16]
Nitromethane	1-Phenyl-1-Butanone	298.1	1.92	2.35	22.4%	1.27	-33.9%	[34]
Nitromethane	1-Propanol	298.2	8.48	10.44	23.1%	8.03	-5.3%	[16]
Nitromethane	2,2,4-Trimethylpentane	293.2	38.50	38.20	-0.8%	20.18	-47.6%	[10]
Nitromethane	2,2,4-Trimethylpentane	298.2	32.55	33.83	3.9%	18.45	-43.3%	[16]
Nitromethane	2,6-Dimethylpyridine	298.2	1.73	1.80	4.0%	M.P.	N.A.	[16]
Nitromethane	2-Methyl-2-Propanol	298.2	8.81	6.08	-31.0%	12.55	42.5%	[16]
Nitromethane	Acetic Acid	298.2	2.50	5.33	113.2%	M.P.	N.A.	[16]
Nitromethane	Acetone	298.2	0.91	0.81	-11.0%	0.87	-4.4%	[16]
Nitromethane	Acetone	298.2	0.88	0.81	-8.1%	0.87	-1.2%	194
Nitromethane	Acetone	298.3	1.10	0.81	-26.4%	0.87	-20.9%	[17]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Nitromethane	Acetone	348.2	0.91	0.88	-3.8%	0.92	0.6%	194
Nitromethane	Acetonitrile	298.2	0.97	0.99	1.8%	0.96	-1.3%	192
Nitromethane	Acetonitrile	348.2	0.96	0.99	2.6%	0.96	-0.5%	192
Nitromethane	Acetonitrile	398.2	0.97	0.99	1.6%	0.95	-2.5%	192
Nitromethane	Acetophenone	298.2	1.21	1.51	24.8%	0.96	-20.7%	[16]
Nitromethane	Aniline	298.2	1.14	1.35	18.4%	M.P.	N.A.	[16]
Nitromethane	Anisole	298.2	1.99	2.18	9.5%	1.26	-36.7%	[16]
Nitromethane	Benzene	318.2	3.48	3.65	4.9%	2.99	-14.1%	[12]
Nitromethane	Benzonitrile	298.2	1.21	1.02	-15.7%	M.G.	N.A.	[16]
Nitromethane	Benzyl Alcohol	298.2	2.57	3.00	16.7%	2.77	7.8%	[16]
Nitromethane	Bromobenzene	298.2	4.40	3.69	-16.1%	2.37	-46.1%	[16]
Nitromethane	Bromoethane	298.2	3.78	4.13	9.3%	6.68	76.7%	[16]
Nitromethane	Butyl Ether	298.2	7.56	9.16	21.2%	3.94	-47.9%	[16]
Nitromethane	Butyronitrile	298.2	1.12	0.97	-13.4%	M.P.	N.A.	[16]
Nitromethane	Carbon Disulfide	298.2	38.09	48.98	28.6%	9.65	-74.7%	[16]
Nitromethane	Carbon Disulfide	298.3	41.30	48.88	18.4%	9.63	-76.7%	[17]
Nitromethane	Carbon Disulfide	308.4	34.50	39.56	14.7%	8.04	-76.7%	[17]
Nitromethane	Carbon Disulfide	318.7	30.60	32.49	6.2%	6.77	-77.9%	[17]
Nitromethane	Carbon Tetrachloride	293.2	15.20	17.67	16.3%	12.40	-18.4%	[10]
Nitromethane	Carbon Tetrachloride	298.2	15.05	16.19	7.6%	11.77	-21.8%	[16]
Nitromethane	Carbon Tetrachloride	314.9	11.70	12.43	6.2%	9.99	-14.6%	[12]
Nitromethane	Carbon Tetrachloride	328.3	10.70	10.33	-3.5%	8.87	-17.1%	[12]
Nitromethane	Carbon Tetrachloride	340.2	9.10	8.91	-2.1%	8.04	-11.6%	[12]
Nitromethane	Carbon Tetrachloride	349.1	8.40	8.05	-4.2%	7.50	-10.7%	[12]
Nitromethane	Chlorobenzene	298.2	3.97	3.83	-3.5%	3.87	-2.5%	[16]
Nitromethane	Chloroform	298.2	2.58	2.73	5.8%	M.P.	N.A.	[16]
Nitromethane	Chloroform	319.8	2.90	2.46	-15.2%	M.P.	N.A.	[12]
Nitromethane	Chloroform	331.9	2.60	2.34	-10.0%	M.P.	N.A.	[12]
Nitromethane	Cyclohexane	298.2	44.90	46.50	3.6%	38.81	-13.6%	[16]
Nitromethane	Cyclohexanone	298.2	0.95	1.16	22.1%	1.51	58.9%	[16]
Nitromethane	Dichloromethane	298.1	2.16	1.95	-9.8%	2.03	-6.1%	191
Nitromethane	Dichloromethane	298.2	1.90	1.95	2.6%	2.03	6.8%	[16]
Nitromethane	Dichloromethane	348.0	1.78	1.71	-3.8%	1.75	-1.6%	191
Nitromethane	Dichloromethane	398.1	1.73	1.55	-10.4%	1.41	-18.5%	191
Nitromethane	Diethyl Ether	298.2	3.93	5.08	29.3%	3.14	-20.1%	[16]
Nitromethane	Diiodomethane	298.2	11.22	11.33	1.0%	M.G.	N.A.	[16]
Nitromethane	Diisopropyl Ether	298.2	5.57	7.80	40.0%	5.34	-4.1%	[16]
Nitromethane	Dimethyl Sulfoxide	298.2	0.57	0.39	-31.6%	M.P.	N.A.	[16]
Nitromethane	Ethanol	298.2	6.82	7.13	4.5%	7.78	14.1%	[16]
Nitromethane	Ethanol	298.2	7.77	7.13	-8.2%	7.78	0.1%	196
Nitromethane	Ethanol	348.2	4.67	5.20	11.4%	4.30	-7.9%	196
Nitromethane	Ethanol	398.2	2.97	3.98	33.9%	3.11	4.6%	196
Nitromethane	Ethyl Acetate	298.2	1.26	1.55	23.0%	1.26	0.0%	[16]
Nitromethane	Ethyl Acetate	298.2	1.20	1.55	29.4%	1.26	5.2%	193
Nitromethane	Ethyl Acetate	311.7	1.62	1.51	-6.8%	1.27	-21.6%	[12]
Nitromethane	Ethyl Acetate	328.4	1.29	1.47	14.0%	1.28	-0.8%	[17]
Nitromethane	Ethyl Acetate	330.5	1.47	1.46	-0.7%	1.28	-12.9%	[12]
Nitromethane	Ethyl Acetate	347.3	1.42	1.42	0.0%	1.30	-8.5%	[12]
Nitromethane	Ethyl Acetate	348.2	1.21	1.42	17.7%	1.30	7.8%	193
Nitromethane	Ethyl Acetate	398.2	1.23	1.32	7.2%	1.31	6.4%	193
Nitromethane	Isopropanol	298.2	9.38	8.00	-14.7%	8.92	-4.9%	[16]
Nitromethane	M-Cresol	298.2	2.03	1.67	-17.7%	M.P.	N.A.	[16]

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Nitromethane	Methanol	298.2	5.59	6.06	8.4%	5.12	-8.4%	[16]
Nitromethane	Methanol	298.2	5.68	6.06	6.7%	5.12	-9.8%	195
Nitromethane	Methanol	308.7	5.05	5.78	14.5%	4.79	-5.1%	[17]
Nitromethane	Methanol	318.5	4.70	5.52	17.4%	4.52	-3.8%	[17]
Nitromethane	Methanol	328.5	4.24	5.27	24.3%	4.28	0.9%	[17]
Nitromethane	Methanol	337.0	3.83	5.06	32.1%	4.10	7.0%	[17]
Nitromethane	Methanol	348.2	4.14	4.79	15.6%	3.90	-5.9%	195
Nitromethane	Methanol	388.2	3.29	3.97	20.8%	3.39	3.2%	195
Nitromethane	Methyl Ethyl Ketone	314.7	1.25	1.11	-11.2%	1.00	-20.0%	[12]
Nitromethane	Methyl Ethyl Ketone	333.3	1.23	1.11	-9.8%	1.01	-17.9%	[12]
Nitromethane	Methyl Ethyl Ketone	350.2	1.20	1.11	-7.5%	1.03	-14.2%	[12]
Nitromethane	Methylcyclohexane	343.2	22.60	17.03	-24.6%	15.97	-29.3%	[83]
Nitromethane	Methylcyclohexane	353.2	19.10	14.60	-23.6%	14.25	-25.4%	[83]
Nitromethane	N,N-Dimethylformamide	298.2	0.56	0.77	37.5%	0.53	-5.4%	[16]
Nitromethane	N-Decane	298.2	30.81	35.67	15.8%	15.73	-48.9%	[16]
Nitromethane	N-Heptane	293.2	41.00	41.68	1.7%	22.40	-45.4%	[10]
Nitromethane	N-Hexadecane	298.2	26.94	33.05	22.7%	11.43	-57.6%	[6]
Nitromethane	N-Hexadecane	298.2	22.91	33.05	44.3%	11.43	-50.1%	[16]
Nitromethane	N-Hexane	298.2	39.73	37.09	-6.6%	23.24	-41.5%	[16]
Nitromethane	N-Hexane	322.9	23.90	22.01	-7.9%	16.80	-29.7%	[12]
Nitromethane	N-Hexane	332.3	19.90	18.57	-6.7%	15.53	-22.0%	[12]
Nitromethane	N-Hexane	340.9	17.80	16.08	-9.7%	14.71	-17.4%	[12]
Nitromethane	Nitrobenzene	298.2	1.40	1.38	-1.4%	1.42	1.4%	[16]
Nitromethane	N-Octane	293.2	39.50	41.26	4.5%	20.22	-48.8%	[10]
Nitromethane	N-Octane	313.2	24.60	26.10	6.1%	14.85	-39.6%	[36]
Nitromethane	N-Octane	333.2	21.40	17.82	-16.7%	12.27	-42.7%	[36]
Nitromethane	N-Pentane	298.2	46.76	37.11	-20.6%	27.42	-41.4%	[16]
Nitromethane	P-Xylene	298.2	4.16	6.16	48.1%	4.32	3.8%	[16]
Nitromethane	Pyridine	298.2	1.27	1.43	12.6%	M.P.	N.A.	[16]
Nitromethane	Tetrahydrofuran	298.2	1.33	2.13	60.2%	2.46	85.0%	[16]
Nitromethane	Toluene	293.2	4.41	5.62	27.4%	3.78	-14.3%	[10]
Nitromethane	Toluene	298.2	3.81	5.34	40.2%	3.70	-2.9%	[16]
Nitromethane	Toluene	343.2	3.92	3.65	-6.9%	3.19	-18.6%	[83]
Nitromethane	Toluene	353.2	3.69	3.41	-7.6%	3.10	-16.0%	[83]
Nitromethane	Triethylamine	298.2	10.63	10.83	1.9%	M.P.	N.A.	[16]
Nitromethane	Triethylamine	348.7	6.70	5.92	-11.6%	M.P.	N.A.	[12]
N-Methyl-2-Pyrrolidone	Benzene	333.3	0.83	1.40	68.8%	1.20	44.7%	41
N-Methyl-2-Pyrrolidone	Benzene	354.2	0.88	1.38	56.5%	1.23	39.5%	41
N-Methyl-2-Pyrrolidone	Chloroform	323.2	0.05	0.05	-1.2%	M.P.	N.A.	323
N-Methyl-2-Pyrrolidone	Chloroform	373.2	0.16	0.12	-26.6%	M.P.	N.A.	323
N-Methyl-2-Pyrrolidone	Cyclohexane	333.3	17.79	15.93	-10.5%	7.90	-55.6%	238
N-Methyl-2-Pyrrolidone	Cyclohexane	354.2	12.90	11.96	-7.3%	6.73	-47.8%	238
N-Methyl-2-Pyrrolidone	N-Decane	313.2	15.10	21.91	45.1%	9.31	-38.3%	[42]
N-Methyl-2-Pyrrolidone	N-Decane	333.2	12.60	15.68	24.4%	7.62	-39.5%	[42]
N-Methyl-2-Pyrrolidone	N-Hexane	333.3	23.34	19.68	-15.7%	12.62	-45.9%	238
N-Methyl-2-Pyrrolidone	N-Nonane	313.2	16.70	22.82	36.6%	10.16	-39.2%	[42]
N-Methyl-2-Pyrrolidone	N-Nonane	333.2	13.70	16.33	19.2%	8.32	-39.3%	[42]
N-Methyl-2-Pyrrolidone	N-Octane	313.2	17.80	24.17	35.8%	11.31	-36.5%	[42]
N-Methyl-2-Pyrrolidone	N-Octane	333.2	14.40	17.26	19.9%	9.26	-35.7%	[42]
N-Methyl-2-Pyrrolidone	P-Xylene	373.2	2.78	2.29	-17.5%	1.60	-42.4%	323
N-Methyl-2-Pyrrolidone	P-Xylene	473.2	1.99	1.75	-12.0%	1.41	-29.1%	323
N-Methyl-2-Pyrrolidone	Toluene	363.3	2.32	1.71	-26.4%	1.45	-37.6%	238

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N-Methyl-2-Pyrrolidone	Toluene	383.4	2.47	1.65	-33.2%	1.45	-41.3%	238
N-Methylacetamide	Aniline	413.5	1.26	0.95	-24.4%	0.62	-50.7%	327
N-Methylacetamide	Ethanol	313.2	0.82	0.69	-16.4%	0.91	10.3%	253
N-Methylacetamide	Methanol	398.6	0.70	0.46	-34.0%	0.50	-28.3%	328
N-Methylacetamide	Phenol	413.5	0.06	0.09	50.0%	M.P.	N.A.	327
N-Methylacetamide	Pyridine	398.6	2.12	1.36	-35.7%	1.62	-23.4%	328
N-Methylformamide	Ethanol	303.2	1.46	1.49	2.1%	M.P.	N.A.	254
N-Methylformamide	Ethanol	313.2	1.43	1.45	1.7%	M.P.	N.A.	254
N-Methylformamide	Methanol	303.2	1.18	0.88	-25.6%	M.P.	N.A.	255
N-Methylformamide	Methanol	313.2	1.14	0.88	-22.9%	M.P.	N.A.	255
N-Nonane	1,2-Dichloroethane	298.2	7.16	5.73	-20.0%	5.12	-28.5%	[50]
N-Nonane	1,4-Dioxane	298.2	10.42	6.44	-38.2%	8.69	-16.6%	[50]
N-Nonane	1-Butanol	298.2	8.19	8.32	1.6%	6.90	-15.8%	[50]
N-Nonane	1-Hexene	298.2	1.15	0.95	-17.4%	1.01	-12.2%	[50]
N-Nonane	1-Octanol	298.2	3.78	4.21	11.4%	3.27	-13.5%	[50]
N-Nonane	1-Octene	298.2	1.19	1.01	-15.1%	1.04	-12.6%	[50]
N-Nonane	1-Pentanol	353.2	4.45	4.96	11.5%	4.36	-2.0%	[21]
N-Nonane	1-Pentanol	373.2	4.47	4.44	-0.7%	3.87	-13.4%	[21]
N-Nonane	1-Propanol	298.2	11.83	10.92	-7.7%	10.01	-15.4%	[50]
N-Nonane	2,2,4-Trimethylpentane	298.2	1.16	1.18	1.7%	1.00	-13.8%	[50]
N-Nonane	2-Heptanone	298.2	3.09	2.99	-3.2%	3.06	-1.0%	[50]
N-Nonane	2-Pentanone	298.2	4.29	4.30	0.2%	4.59	7.0%	[50]
N-Nonane	Acetic Acid	298.2	37.62	32.16	-14.5%	25.77	-31.5%	[50]
N-Nonane	Acetone	298.2	12.86	11.58	-10.0%	9.66	-24.9%	[50]
N-Nonane	Acetonitrile	298.2	78.75	77.67	-1.4%	53.81	-31.7%	[50]
N-Nonane	Acetophenone	298.2	9.75	9.70	-0.5%	16.67	71.0%	[50]
N-Nonane	Anisole	298.2	4.88	4.75	-2.7%	3.47	-28.9%	[50]
N-Nonane	Benzene	298.2	2.37	2.06	-13.1%	2.10	-11.4%	[50]
N-Nonane	Benzonitrile	298.2	9.63	11.19	16.2%	M.G.	N.A.	[50]
N-Nonane	Benzyl Alcohol	298.2	26.51	24.76	-6.6%	16.88	-36.3%	[50]
N-Nonane	Butyl Acetate	298.2	3.09	2.76	-10.7%	3.66	18.4%	[50]
N-Nonane	Butyronitrile	298.2	11.11	11.01	-0.9%	9.48	-14.7%	[50]
N-Nonane	Carbon Disulfide	298.2	1.98	1.67	-15.7%	1.68	-15.2%	[50]
N-Nonane	Carbon Tetrachloride	298.2	1.28	1.16	-9.4%	1.20	-6.3%	[50]
N-Nonane	Chlorobenzene	298.2	2.18	2.23	2.3%	2.50	14.7%	[50]
N-Nonane	Chloroform	298.2	2.07	2.19	5.8%	2.00	-3.4%	[50]
N-Nonane	Cyclohexane	298.2	1.01	0.96	-5.0%	1.02	1.0%	[50]
N-Nonane	Cyclohexanone	298.2	5.96	5.86	-1.7%	3.92	-34.2%	[50]
N-Nonane	Dichloromethane	298.2	4.16	3.73	-10.3%	4.00	-3.8%	[50]
N-Nonane	Dimethyl Sulfoxide	298.2	264.98	230.17	-13.1%	228.91	-13.6%	[50]
N-Nonane	Ethanol	298.2	19.65	23.80	21.1%	18.07	-8.0%	[50]
N-Nonane	Ethanol	301.1	20.80	23.46	12.8%	17.82	-14.3%	[48]
N-Nonane	Ethanol	320.9	19.80	20.61	4.1%	15.80	-20.2%	[48]
N-Nonane	Ethanol	320.9	18.90	20.61	9.0%	15.80	-16.4%	[48]
N-Nonane	Ethanol	355.2	15.50	15.18	-2.1%	11.48	-25.9%	[48]
N-Nonane	Ethyl Acetate	298.2	5.43	4.77	-12.2%	5.15	-5.2%	[50]
N-Nonane	Isopropanol	298.2	10.85	11.04	1.8%	7.68	-29.2%	[50]
N-Nonane	Methanol	298.2	64.79	71.61	10.5%	51.00	-21.3%	[50]
N-Nonane	Methyl Acetate	298.2	10.34	9.61	-7.1%	9.65	-6.7%	[50]
N-Nonane	Methyl Ethyl Ketone	298.2	6.03	6.05	0.3%	6.25	3.6%	[50]
N-Nonane	N-Decane	298.2	1.18	1.00	-15.3%	1.00	-15.3%	[50]
N-Nonane	N-Dodecane	298.2	1.06	0.99	-6.6%	0.99	-6.6%	[50]

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N-Nonane	N-Heptane	298.2	1.05	0.99	-5.7%	1.00	-4.8%	[50]
N-Nonane	N-Hexadecane	298.2	0.99	0.93	-6.1%	0.96	-3.0%	[50]
N-Nonane	N-Hexadecane	298.2	1.02	0.93	-8.9%	0.96	-6.0%	[6]
N-Nonane	N-Hexane	298.2	1.02	0.99	-2.9%	0.99	-2.9%	[50]
N-Nonane	Nitrobenzene	298.2	12.48	12.57	0.7%	12.18	-2.4%	[50]
N-Nonane	Nitromethane	298.2	190.86	140.20	-26.5%	143.64	-24.7%	[50]
N-Nonane	N-Methyl-2-Pyrrolidone	298.2	26.69	25.72	-3.6%	19.36	-27.5%	[50]
N-Nonane	N-Methylformamide	298.2	115.83	120.07	3.7%	M.P.	N.A.	[50]
N-Nonane	N-Nonane	298.2	1.14	1.00	-12.3%	1.00	-12.3%	[50]
N-Nonane	N-Octane	298.2	1.09	1.00	-8.3%	1.00	-8.3%	[50]
N-Nonane	N-Pentane	298.2	1.21	1.00	-17.4%	0.99	-18.2%	[50]
N-Nonane	Propionitrile	298.2	22.47	23.55	4.8%	14.02	-37.6%	[50]
N-Nonane	P-Xylene	298.2	1.66	1.47	-11.4%	1.31	-21.1%	[50]
N-Nonane	Pyridine	298.2	9.69	8.82	-9.0%	8.30	-14.3%	[50]
N-Nonane	Squalane	298.2	0.68	0.75	10.3%	0.80	17.6%	[50]
N-Nonane	Tetrahydrofuran	298.2	2.45	2.21	-9.8%	1.95	-20.4%	[50]
N-Nonane	Toluene	298.2	1.84	1.79	-2.7%	1.53	-16.8%	[50]
N-Nonane	Triethylamine	298.2	1.10	1.14	3.6%	1.05	-4.5%	[50]
N-Octane	1,1-Dichloroethane	298.2	6.03	5.44	-9.8%	1.93	-68.0%	[16]
N-Octane	1,2-Dichloroethane	298.2	6.43	5.36	-16.6%	4.54	-29.4%	[50]
N-Octane	1,4-Dioxane	298.2	8.90	5.98	-32.8%	7.54	-15.3%	[50]
N-Octane	1,4-Dioxane	298.2	7.40	5.98	-19.2%	7.54	1.9%	[16]
N-Octane	1,4-Dioxane	353.2	4.23	3.84	-9.3%	4.38	3.5%	198
N-Octane	1,5-Dimethyl-2-Pyrrolidinone	298.2	11.10	12.32	11.0%	M.G.	N.A.	[29]
N-Octane	1,5-Dimethyl-2-Pyrrolidinone	308.2	10.60	10.86	2.5%	M.G.	N.A.	[29]
N-Octane	1,5-Dimethyl-2-Pyrrolidinone	318.2	10.10	9.68	-4.2%	M.G.	N.A.	[29]
N-Octane	1-Butanol	298.2	6.86	7.09	3.4%	6.12	-10.8%	[50]
N-Octane	1-Butanol	298.2	6.39	7.09	11.0%	6.12	-4.2%	[16]
N-Octane	1-Butanol	308.2	6.26	6.84	9.3%	5.97	-4.6%	[30]
N-Octane	1-Butanol	318.2	6.01	6.55	9.0%	5.79	-3.7%	[30]
N-Octane	1-Butanol	328.2	6.64	6.24	-6.0%	5.59	-15.8%	[30]
N-Octane	1-Ethylpyrrolidin-2-One	298.2	11.80	12.07	2.3%	5.54	-53.1%	[29]
N-Octane	1-Ethylpyrrolidin-2-One	308.2	10.50	10.66	1.5%	5.25	-50.0%	[29]
N-Octane	1-Ethylpyrrolidin-2-One	318.2	9.43	9.51	0.8%	4.97	-47.3%	[29]
N-Octane	1-Hexene	298.2	1.18	0.97	-17.8%	1.03	-12.7%	[50]
N-Octane	1-Octanol	293.4	3.05	3.77	23.6%	3.03	-0.7%	[31]
N-Octane	1-Octanol	298.2	3.38	3.68	8.9%	3.02	-10.7%	[50]
N-Octane	1-Octanol	298.2	3.18	3.68	15.7%	3.02	-5.0%	[16]
N-Octane	1-Octanol	298.2	3.36	3.68	9.5%	3.02	-10.1%	[32]
N-Octane	1-Octanol	303.5	3.17	3.58	12.9%	2.99	-5.7%	[31]
N-Octane	1-Octanol	313.6	3.14	3.41	8.6%	2.94	-6.4%	[31]
N-Octane	1-Octanol	323.4	2.90	3.24	11.7%	2.88	-0.7%	[31]
N-Octane	1-Octene	298.2	1.13	1.01	-10.6%	1.05	-7.1%	[50]
N-Octane	1-Pentanol	308.2	5.80	5.44	-6.2%	4.68	-19.3%	[30]
N-Octane	1-Pentanol	313.2	3.94	5.33	35.3%	4.63	17.5%	[33]
N-Octane	1-Pentanol	318.2	5.42	5.22	-3.7%	4.57	-15.7%	[30]
N-Octane	1-Pentanol	328.2	5.30	5.00	-5.7%	4.43	-16.4%	[30]
N-Octane	1-Phenyl-1-Butanone	298.1	4.45	4.95	11.2%	4.72	6.1%	[34]
N-Octane	1-Propanol	298.2	9.52	9.26	-2.7%	8.67	-8.9%	[50]
N-Octane	1-Propanol	298.2	8.94	9.26	3.6%	8.67	-3.0%	[16]

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N-Octane	1-Propanol	308.2	8.36	8.96	7.2%	8.40	0.5%	[47]
N-Octane	1-Propanol	358.2	7.90	6.84	-13.5%	6.38	-19.3%	336
N-Octane	1-Propanol	363.2	6.64	6.63	-0.1%	6.13	-7.6%	336
N-Octane	2,2,4-Trimethylpentane	298.2	1.11	1.12	0.9%	1.00	-9.9%	[50]
N-Octane	2,2,4-Trimethylpentane	298.2	1.02	1.12	9.8%	1.00	-2.0%	[16]
N-Octane	2,6-Dimethylpyridine	298.2	2.60	3.50	34.6%	1.71	-34.2%	[16]
N-Octane	2-Heptanone	298.2	2.72	2.70	-0.7%	2.85	4.8%	[50]
N-Octane	2-Methyl-2-Propanol	298.2	5.73	6.16	7.5%	3.86	-32.6%	[16]
N-Octane	2-Methyl-2-Propanol	313.2	4.07	5.70	40.1%	3.72	-8.6%	259
N-Octane	2-Pentanone	298.2	3.70	3.87	4.6%	4.17	12.7%	[50]
N-Octane	2-Pyrrolidone	303.2	73.33	95.15	29.8%	M.G.	N.A.	[35]
N-Octane	2-Pyrrolidone	313.2	65.83	75.75	15.1%	M.G.	N.A.	[35]
N-Octane	2-Pyrrolidone	323.2	60.27	61.17	1.5%	M.G.	N.A.	[35]
N-Octane	2-Pyrrolidone	333.2	54.98	50.06	-8.9%	M.G.	N.A.	[35]
N-Octane	Acetic Acid	298.2	29.01	25.27	-12.9%	19.18	-33.9%	[50]
N-Octane	Acetic Acid	298.2	26.60	25.27	-5.0%	19.18	-27.9%	[16]
N-Octane	Acetone	298.2	10.58	9.47	-10.5%	8.29	-21.6%	[50]
N-Octane	Acetone	298.2	10.29	9.47	-8.0%	8.29	-19.4%	[16]
N-Octane	Acetone	298.3	11.04	9.46	-14.3%	8.28	-25.0%	[17]
N-Octane	Acetone	308.2	9.75	8.35	-14.4%	7.44	-23.7%	[17]
N-Octane	Acetone	318.4	7.83	7.42	-5.2%	6.69	-14.6%	[17]
N-Octane	Acetone	328.4	7.06	6.67	-5.5%	6.05	-14.3%	[17]
N-Octane	Acetonitrile	298.2	46.90	54.98	17.2%	42.17	-10.1%	[36]
N-Octane	Acetonitrile	298.2	56.51	54.98	-2.7%	42.17	-25.4%	[50]
N-Octane	Acetonitrile	298.2	55.54	54.98	-1.0%	42.17	-24.1%	[16]
N-Octane	Acetophenone	298.2	8.58	8.29	-3.4%	13.79	60.7%	[50]
N-Octane	Acetophenone	298.2	7.60	8.29	9.1%	13.79	81.4%	[16]
N-Octane	Aniline	298.2	37.74	35.93	-4.8%	35.23	-6.7%	[16]
N-Octane	Anisole	298.2	4.52	4.40	-2.7%	3.23	-28.5%	[50]
N-Octane	Anisole	298.2	4.03	4.40	9.2%	3.23	-19.9%	[16]
N-Octane	Benzene	298.2	2.31	2.10	-9.1%	2.12	-8.2%	[50]
N-Octane	Benzene	298.2	2.17	2.10	-3.2%	2.12	-2.3%	[16]
N-Octane	Benzonitrile	298.2	8.28	9.36	13.0%	M.G.	N.A.	[50]
N-Octane	Benzonitrile	298.2	7.69	9.36	21.7%	M.G.	N.A.	[16]
N-Octane	Benzyl Alcohol	298.2	21.00	19.85	-5.5%	14.21	-32.3%	[50]
N-Octane	Benzyl Alcohol	298.2	18.55	19.85	7.0%	14.21	-23.4%	[16]
N-Octane	Bromobenzene	298.2	2.66	2.55	-4.1%	3.22	21.1%	[16]
N-Octane	Bromoethane	298.2	2.22	2.05	-7.7%	1.43	-35.6%	[16]
N-Octane	Butyl Acetate	298.2	2.78	2.55	-8.3%	3.37	21.2%	[50]
N-Octane	Butyl Ether	298.2	1.13	1.22	8.0%	1.10	-2.7%	[5]
N-Octane	Butyronitrile	298.2	9.29	9.22	-0.8%	7.87	-15.3%	[50]
N-Octane	Butyronitrile	298.2	8.96	9.22	2.9%	7.87	-12.2%	[16]
N-Octane	Carbon Disulfide	298.2	2.16	1.93	-10.6%	1.95	-9.7%	[50]
N-Octane	Carbon Disulfide	298.2	2.04	1.93	-5.4%	1.95	-4.4%	[16]
N-Octane	Carbon Tetrachloride	298.2	1.33	1.23	-7.5%	1.24	-6.8%	[50]
N-Octane	Carbon Tetrachloride	298.2	1.23	1.23	0.0%	1.24	0.8%	[16]
N-Octane	Carbon Tetrachloride	313.2	1.19	1.19	-0.1%	1.20	0.7%	93
N-Octane	Chlorobenzene	298.2	2.28	2.24	-1.8%	2.57	12.7%	[50]
N-Octane	Chlorobenzene	298.2	2.19	2.24	2.3%	2.57	17.4%	[16]
N-Octane	Chloroform	298.2	2.06	2.17	5.3%	1.99	-3.4%	[50]
N-Octane	Chloroform	298.2	2.07	2.17	4.8%	1.99	-3.9%	[16]
N-Octane	Cyclohexane	298.2	1.13	1.03	-8.8%	1.05	-7.1%	[50]

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N-Octane	Cyclohexane	298.2	1.09	1.03	-5.5%	1.05	-3.7%	[16]
N-Octane	Cyclohexanone	298.2	5.33	5.24	-1.7%	3.63	-31.9%	[50]
N-Octane	Cyclohexanone	298.2	4.84	5.24	8.3%	3.63	-25.0%	[16]
N-Octane	Dichloromethane	298.2	3.95	3.63	-8.1%	3.54	-10.4%	[50]
N-Octane	Dichloromethane	298.2	4.14	3.63	-12.3%	3.54	-14.5%	[16]
N-Octane	Diethyl Ether	298.2	1.53	1.67	9.2%	1.27	-17.0%	[16]
N-Octane	Diethyl Phthalate	303.2	6.86	7.32	6.7%	M.G.	N.A.	[39]
N-Octane	Diethyl Phthalate	313.2	6.34	6.61	4.3%	M.G.	N.A.	[39]
N-Octane	Diethyl Phthalate	323.2	5.95	6.02	1.2%	M.G.	N.A.	[39]
N-Octane	Diethyl Phthalate	333.2	5.55	5.52	-0.5%	M.G.	N.A.	[39]
N-Octane	Diiodomethane	298.2	56.91	58.56	2.9%	M.G.	N.A.	[16]
N-Octane	Diisopropyl Ether	298.2	1.34	1.29	-3.7%	1.08	-19.4%	[16]
N-Octane	Dimethyl Sulfoxide	283.2	200.00	259.75	29.9%	240.80	20.4%	[40]
N-Octane	Dimethyl Sulfoxide	298.2	171.68	153.64	-10.5%	159.60	-7.0%	[50]
N-Octane	Epsilon-Caprolactone	303.2	19.90	21.99	10.5%	M.G.	N.A.	[41]
N-Octane	Epsilon-Caprolactone	318.2	17.70	17.28	-2.4%	M.G.	N.A.	[41]
N-Octane	Epsilon-Caprolactone	333.2	15.70	13.98	-11.0%	M.G.	N.A.	[41]
N-Octane	Ethanol	298.2	16.12	18.89	17.2%	14.99	-7.0%	[50]
N-Octane	Ethanol	298.2	15.47	18.89	22.1%	14.99	-3.1%	[16]
N-Octane	Ethanol	322.2	14.50	16.46	13.5%	13.18	-9.1%	[48]
N-Octane	Ethanol	338.0	13.10	14.59	11.4%	11.71	-10.6%	[48]
N-Octane	Ethanol	343.2	14.28	13.98	-2.1%	11.19	-21.7%	336
N-Octane	Ethanol	353.7	13.00	12.78	-1.7%	10.12	-22.2%	[48]
N-Octane	Ethyl Acetate	298.2	4.83	4.22	-12.6%	4.44	-8.1%	[50]
N-Octane	Ethyl Acetate	298.2	4.68	4.22	-9.8%	4.44	-5.1%	[16]
N-Octane	Ethyl Acetate	328.4	3.59	3.41	-5.0%	3.42	-4.7%	[17]
N-Octane	Ethyl Acetate	338.4	3.34	3.21	-3.9%	3.17	-5.1%	[17]
N-Octane	Ethyl Acetate	349.1	3.06	3.02	-1.3%	2.94	-3.9%	[17]
N-Octane	Ethyl Benzoate	313.2	3.38	3.51	3.8%	M.G.	N.A.	[41]
N-Octane	Ethyl Benzoate	323.2	3.23	3.30	2.2%	M.G.	N.A.	[41]
N-Octane	Ethyl Benzoate	333.2	3.08	3.12	1.3%	M.G.	N.A.	[41]
N-Octane	Ethyl Benzoate	343.2	2.96	2.96	0.0%	M.G.	N.A.	[41]
N-Octane	Isopropanol	298.2	9.60	9.10	-5.2%	6.74	-29.8%	[50]
N-Octane	Isopropanol	298.2	9.22	9.10	-1.3%	6.74	-26.9%	[16]
N-Octane	Isopropanol	308.2	9.94	8.73	-12.2%	6.54	-34.2%	[47]
N-Octane	Isopropanol	353.2	6.28	6.77	7.8%	5.19	-17.4%	225
N-Octane	M-Cresol	298.2	11.77	13.40	13.8%	11.82	0.4%	[16]
N-Octane	Methanol	298.2	48.02	52.94	10.2%	38.77	-19.3%	[50]
N-Octane	Methanol	298.2	45.86	52.94	15.4%	38.77	-15.5%	[16]
N-Octane	Methanol	308.7	43.20	48.86	13.1%	36.05	-16.6%	[17]
N-Octane	Methanol	318.5	39.70	44.56	12.2%	33.73	-15.0%	[17]
N-Octane	Methanol	328.5	35.90	40.00	11.4%	31.52	-12.2%	[17]
N-Octane	Methanol	337.0	32.30	36.20	12.1%	29.76	-7.9%	[17]
N-Octane	Methyl Acetate	298.2	8.53	7.92	-7.2%	7.75	-9.1%	[50]
N-Octane	Methyl Ethyl Ketone	298.2	5.28	5.30	0.4%	5.55	5.1%	[50]
N-Octane	Methyl Ethyl Ketone	298.2	5.44	5.30	-2.6%	5.55	2.0%	[16]
N-Octane	Methyl Isobutyl Ketone	328.2	2.93	2.61	-10.9%	2.89	-1.4%	[49]
N-Octane	Methyl Isobutyl Ketone	348.2	2.52	2.39	-5.2%	2.64	4.8%	[49]
N-Octane	Methyl Isobutyl Ketone	388.2	1.98	2.06	4.0%	2.24	13.1%	[49]
N-Octane	N,N-Diethylacetamide	303.2	6.64	7.14	7.5%	2.45	-63.1%	[39]
N-Octane	N,N-Diethylacetamide	313.2	6.14	6.47	5.4%	2.33	-62.1%	[39]
N-Octane	N,N-Diethylacetamide	323.2	5.75	5.90	2.6%	2.24	-61.0%	[39]

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N-Octane	N,N-Diethylacetamide	333.2	5.32	5.43	2.1%	2.16	-59.4%	[39]
N-Octane	N,N-Dimethylformamide	283.2	45.20	36.15	-20.0%	30.92	-31.6%	[40]
N-Octane	N,N-Dimethylformamide	298.2	26.56	26.60	0.2%	24.56	-7.5%	[16]
N-Octane	N-Decane	298.2	1.05	0.99	-5.7%	1.00	-4.8%	[50]
N-Octane	N-Decane	298.2	1.02	0.99	-2.9%	1.00	-2.0%	[16]
N-Octane	N-Dodecane	298.2	1.04	0.98	-5.8%	0.98	-5.8%	[50]
N-Octane	N-Ethylacetamide	303.2	13.80	14.88	7.8%	M.G.	N.A.	[39]
N-Octane	N-Ethylacetamide	313.2	13.30	13.76	3.5%	M.G.	N.A.	[39]
N-Octane	N-Ethylacetamide	323.2	12.90	12.69	-1.6%	M.G.	N.A.	[39]
N-Octane	N-Ethylacetamide	333.2	12.50	11.70	-6.4%	M.G.	N.A.	[39]
N-Octane	N-Formylmorpholine	313.3	54.20	57.57	6.2%	M.G.	N.A.	[43]
N-Octane	N-Formylmorpholine	332.7	40.70	39.47	-3.0%	M.G.	N.A.	[43]
N-Octane	N-Formylmorpholine	352.5	33.70	28.23	-16.2%	M.G.	N.A.	[43]
N-Octane	N-Formylmorpholine	373.4	26.30	20.77	-21.0%	M.G.	N.A.	[43]
N-Octane	N-Heptane	298.2	1.07	1.00	-6.5%	1.00	-6.5%	[50]
N-Octane	N-Heptane	298.2	1.05	1.00	-4.8%	1.00	-4.8%	[16]
N-Octane	N-Hexadecane	298.2	0.96	0.91	-5.2%	0.94	-2.1%	[50]
N-Octane	N-Hexadecane	298.2	0.98	0.91	-7.1%	0.94	-4.1%	[6]
N-Octane	N-Hexadecane	298.2	0.92	0.91	-1.1%	0.94	2.2%	[16]
N-Octane	N-Hexadecane	453.2	0.89	0.90	1.1%	0.94	5.6%	[71]
N-Octane	N-Hexane	298.2	1.09	0.99	-9.2%	1.00	-8.3%	[50]
N-Octane	N-Hexane	298.2	1.08	0.99	-8.3%	1.00	-7.4%	[16]
N-Octane	Nitrobenzene	298.2	10.91	10.58	-3.0%	10.52	-3.6%	[50]
N-Octane	Nitrobenzene	298.2	9.32	10.58	13.5%	10.52	12.9%	[16]
N-Octane	Nitromethane	298.2	125.57	93.20	-25.8%	100.32	-20.1%	[50]
N-Octane	Nitromethane	298.2	111.20	93.20	-16.2%	100.32	-9.8%	[16]
N-Octane	N-Methyl-2-Pyrrolidone	298.2	21.26	21.26	0.0%	15.71	-26.1%	[50]
N-Octane	N-Methyl-2-Pyrrolidone	323.4	18.90	14.64	-22.5%	13.68	-27.6%	[43]
N-Octane	N-Methyl-2-Pyrrolidone	333.2	16.80	12.92	-23.1%	12.83	-23.6%	[43]
N-Octane	N-Methyl-2-Pyrrolidone	343.4	16.10	11.45	-28.9%	11.94	-25.8%	[43]
N-Octane	N-Methylformamide	298.2	81.27	84.91	4.5%	M.P.	N.A.	[50]
N-Octane	N-Methylformamide	303.2	80.48	78.78	-2.1%	M.P.	N.A.	[35]
N-Octane	N-Methylformamide	313.2	71.89	67.67	-5.9%	M.P.	N.A.	[35]
N-Octane	N-Methylformamide	323.2	64.57	58.05	-10.1%	M.P.	N.A.	[35]
N-Octane	N-Methylformamide	333.2	58.58	49.82	-15.0%	M.P.	N.A.	[35]
N-Octane	N-Nonane	298.2	1.12	1.00	-10.7%	1.00	-10.7%	[50]
N-Octane	N-Octane	298.2	1.07	1.00	-6.5%	1.00	-6.5%	[50]
N-Octane	N-Pentane	298.2	1.22	1.01	-17.2%	1.00	-18.0%	[50]
N-Octane	N-Pentane	298.2	1.18	1.01	-14.4%	1.00	-15.3%	[16]
N-Octane	Phenol	328.2	19.99	19.93	-0.3%	18.47	-7.6%	[14]
N-Octane	Phenol	343.2	16.97	17.58	3.6%	15.53	-8.5%	[14]
N-Octane	Phenol	358.2	15.10	15.42	2.1%	13.06	-13.5%	[14]
N-Octane	Phenol	373.2	14.15	13.51	-4.5%	10.98	-22.4%	[14]
N-Octane	Propionitrile	298.2	17.73	18.73	5.6%	12.21	-31.1%	[50]
N-Octane	Propionitrile	313.2	16.34	14.40	-11.9%	10.44	-36.1%	124
N-Octane	P-Xylene	298.2	1.55	1.48	-4.5%	1.38	-11.0%	[50]
N-Octane	P-Xylene	298.2	1.40	1.48	5.7%	1.38	-1.4%	[16]
N-Octane	P-Xylene	313.2	1.44	1.43	-0.6%	1.34	-6.8%	101
N-Octane	Pyridine	298.2	8.52	7.88	-7.5%	7.96	-6.6%	[50]
N-Octane	Pyridine	298.2	9.17	7.88	-14.1%	7.96	-13.2%	[16]
N-Octane	Pyridine	313.2	7.58	6.62	-12.7%	6.97	-8.0%	588
N-Octane	Pyridine	353.2	4.32	4.51	4.3%	5.12	18.4%	588

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N-Octane	Pyridine	369.8	3.86	3.96	2.6%	4.49	16.3%	588
N-Octane	Squalane	298.2	0.71	0.68	-4.2%	0.78	9.9%	[50]
N-Octane	Tetrahydrofuran	298.2	2.33	2.19	-6.0%	1.95	-16.3%	[50]
N-Octane	Tetrahydrofuran	298.2	1.78	2.19	23.0%	1.95	9.6%	[16]
N-Octane	Toluene	298.2	1.75	1.81	3.4%	1.59	-9.1%	[50]
N-Octane	Toluene	298.2	1.69	1.81	7.1%	1.59	-5.9%	[16]
N-Octane	Toluene	333.2	1.48	1.61	8.5%	1.45	-2.3%	332
N-Octane	Tributyl Phosphate	298.6	2.53	2.77	9.5%	M.G.	N.A.	[27]
N-Octane	Tributyl Phosphate	302.9	2.39	2.70	13.0%	M.G.	N.A.	[27]
N-Octane	Tributyl Phosphate	308.6	2.34	2.60	11.1%	M.G.	N.A.	[27]
N-Octane	Tributyl Phosphate	313.1	2.29	2.54	10.9%	M.G.	N.A.	[27]
N-Octane	Tributyl Phosphate	323.7	2.12	2.39	12.7%	M.G.	N.A.	[27]
N-Octane	Triethylamine	298.2	1.09	1.12	2.8%	1.05	-3.7%	[50]
N-Pentane	1,2-Dichloroethane	293.2	4.79	4.63	-3.3%	3.25	-32.2%	[10]
N-Pentane	1,2-Dichloroethane	298.2	4.50	4.44	-1.3%	3.13	-30.4%	[50]
N-Pentane	1,4-Dioxane	298.2	5.51	4.87	-11.6%	4.87	-11.6%	[50]
N-Pentane	1,5-Dimethyl-2-Pyrrolidinone	298.2	6.95	7.23	4.0%	M.G.	N.A.	[29]
N-Pentane	1,5-Dimethyl-2-Pyrrolidinone	308.2	6.77	6.58	-2.8%	M.G.	N.A.	[29]
N-Pentane	1,5-Dimethyl-2-Pyrrolidinone	318.2	6.58	6.03	-8.4%	M.G.	N.A.	[29]
N-Pentane	1-Butanol	293.2	4.30	4.47	4.0%	4.27	-0.7%	[10]
N-Pentane	1-Butanol	298.2	4.03	4.42	9.7%	4.24	5.2%	[50]
N-Pentane	1-Butanol	308.2	4.12	4.31	4.6%	4.17	1.2%	[30]
N-Pentane	1-Butanol	318.2	3.83	4.18	9.1%	4.08	6.5%	[30]
N-Pentane	1-Butanol	328.2	3.85	4.04	4.9%	3.99	3.6%	[30]
N-Pentane	1-Ethylpyrrolidin-2-One	298.2	7.15	7.30	2.1%	3.82	-46.6%	[29]
N-Pentane	1-Ethylpyrrolidin-2-One	308.2	6.61	6.65	0.6%	3.69	-44.2%	[29]
N-Pentane	1-Ethylpyrrolidin-2-One	318.2	6.13	6.10	-0.5%	3.56	-41.9%	[29]
N-Pentane	1-Hexene	298.2	1.03	1.03	0.0%	1.08	4.9%	[50]
N-Pentane	1-Nitropropane	298.2	5.35	6.40	19.6%	4.82	-9.9%	[50]
N-Pentane	1-Octanol	293.4	2.46	2.51	2.0%	2.33	-5.3%	[31]
N-Pentane	1-Octanol	298.2	2.22	2.47	11.3%	2.32	4.5%	[50]
N-Pentane	1-Octanol	298.2	2.62	2.47	-5.7%	2.32	-11.5%	[32]
N-Pentane	1-Octanol	298.2	2.58	2.47	-4.3%	2.32	-10.1%	[4]
N-Pentane	1-Octanol	303.5	2.42	2.42	0.0%	2.31	-4.5%	[31]
N-Pentane	1-Octanol	313.6	2.39	2.33	-2.5%	2.28	-4.6%	[31]
N-Pentane	1-Octanol	323.4	2.32	2.25	-3.0%	2.25	-3.0%	[31]
N-Pentane	1-Octene	298.2	0.97	1.02	5.2%	1.06	9.3%	[50]
N-Pentane	1-Pentanol	303.5	3.82	3.70	-3.1%	3.43	-10.2%	[33]
N-Pentane	1-Pentanol	308.2	4.31	3.65	-15.3%	3.41	-20.9%	[30]
N-Pentane	1-Pentanol	313.2	3.82	3.60	-5.8%	3.38	-11.5%	[33]
N-Pentane	1-Pentanol	318.2	3.69	3.54	-4.1%	3.35	-9.2%	[30]
N-Pentane	1-Pentanol	323.5	3.68	3.48	-5.4%	3.32	-9.8%	[33]
N-Pentane	1-Pentanol	328.2	3.53	3.43	-2.8%	3.28	-7.1%	[30]
N-Pentane	1-Propanol	298.2	5.11	5.69	11.4%	5.60	9.6%	[50]
N-Pentane	1-Propanol	308.2	5.62	5.55	-1.2%	5.48	-2.5%	[47]
N-Pentane	2,2,4-Trimethylpentane	293.2	0.98	0.95	-3.1%	0.99	1.0%	[10]
N-Pentane	2,2,4-Trimethylpentane	298.2	0.93	0.95	2.2%	0.99	6.5%	[50]
N-Pentane	2-Heptanone	298.2	1.88	1.97	4.8%	2.26	20.2%	[50]
N-Pentane	2-Nitropropane	293.2	6.50	6.04	-7.1%	4.84	-25.5%	[10]
N-Pentane	2-Pentanone	298.2	2.58	2.83	9.7%	3.09	19.8%	[50]

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N-Pentane	2-Pyrrolidone	303.2	31.82	34.87	9.6%	M.G.	N.A.	[35]
N-Pentane	2-Pyrrolidone	313.2	29.29	29.50	0.7%	M.G.	N.A.	[35]
N-Pentane	2-Pyrrolidone	323.2	27.44	25.22	-8.1%	M.G.	N.A.	[35]
N-Pentane	2-Pyrrolidone	333.2	25.43	21.77	-14.4%	M.G.	N.A.	[35]
N-Pentane	Acetic Acid	298.2	11.65	12.43	6.7%	8.03	-31.1%	[50]
N-Pentane	Acetone	238.2	14.79	10.73	-27.5%	8.70	-41.2%	407
N-Pentane	Acetone	258.2	9.61	8.00	-16.8%	7.24	-24.7%	407
N-Pentane	Acetone	298.2	5.98	5.17	-13.5%	5.24	-12.3%	407
N-Pentane	Acetone	298.2	5.14	5.17	0.6%	5.24	1.9%	[50]
N-Pentane	Acetone	303.2	5.77	4.95	-14.2%	5.06	-12.3%	[18]
N-Pentane	Acetone	303.2	5.84	4.95	-15.2%	5.06	-13.4%	[18]
N-Pentane	Acetone	308.2	5.29	4.75	-10.2%	4.88	-7.8%	[75]
N-Pentane	Acetone	318.3	4.51	4.38	-2.9%	4.55	0.9%	[18]
N-Pentane	Acetone	323.2	4.29	4.23	-1.4%	4.40	2.6%	[18]
N-Pentane	Acetonitrile	293.2	26.92	21.73	-19.3%	22.26	-17.3%	[45]
N-Pentane	Acetonitrile	298.2	17.20	19.74	14.8%	20.54	19.4%	[36]
N-Pentane	Acetonitrile	298.2	17.04	19.74	15.8%	20.54	20.5%	[50]
N-Pentane	Acetonitrile	313.2	21.25	15.15	-28.7%	16.35	-23.1%	[45]
N-Pentane	Acetophenone	293.2	6.00	5.50	-8.3%	7.98	33.0%	[10]
N-Pentane	Acetophenone	298.2	5.23	5.26	0.6%	7.70	47.2%	[50]
N-Pentane	Aniline	293.2	19.72	17.59	-10.8%	16.80	-14.8%	[37]
N-Pentane	Aniline	293.2	20.10	17.59	-12.5%	16.80	-16.4%	[10]
N-Pentane	Anisole	293.2	3.64	3.66	0.5%	2.65	-27.2%	[5]
N-Pentane	Anisole	293.2	3.64	3.66	0.5%	2.65	-27.2%	[10]
N-Pentane	Anisole	298.2	3.32	3.54	6.6%	2.59	-22.0%	[50]
N-Pentane	Benzene	293.2	2.25	2.29	1.8%	2.22	-1.3%	[10]
N-Pentane	Benzene	298.2	2.04	2.24	9.8%	2.17	6.4%	[50]
N-Pentane	Benzonitrile	293.2	6.08	5.80	-4.6%	M.G.	N.A.	[10]
N-Pentane	Benzonitrile	298.2	5.16	5.54	7.4%	M.G.	N.A.	[50]
N-Pentane	Benzyl Alcohol	298.2	9.83	10.48	6.6%	8.37	-14.9%	[50]
N-Pentane	Benzyl Alcohol	298.2	11.53	10.48	-9.1%	8.37	-27.4%	[67]
N-Pentane	Butyl Acetate	298.2	1.92	2.02	5.2%	2.60	35.4%	[50]
N-Pentane	Butyl Ether	293.2	1.00	1.11	11.0%	1.06	6.0%	[5]
N-Pentane	Butyronitrile	298.2	4.96	5.46	10.1%	4.51	-9.1%	[50]
N-Pentane	Carbon Disulfide	298.2	2.46	3.07	24.8%	3.11	26.4%	[50]
N-Pentane	Carbon Tetrachloride	298.2	1.33	1.47	10.5%	1.38	3.8%	[50]
N-Pentane	Chlorobenzene	298.2	2.15	2.26	5.1%	2.77	28.8%	[50]
N-Pentane	Chloroform	298.2	1.96	2.13	8.7%	1.98	1.0%	[50]
N-Pentane	Chloroform	298.2	2.13	2.13	0.0%	1.98	-7.0%	[30]
N-Pentane	Cyclohexane	298.2	1.22	1.29	5.7%	1.11	-9.0%	[50]
N-Pentane	Cyclohexanone	293.2	3.97	3.91	-1.5%	2.88	-27.5%	[10]
N-Pentane	Cyclohexanone	298.2	3.69	3.79	2.7%	2.82	-23.6%	[50]
N-Pentane	Dichloromethane	298.2	3.22	3.34	3.7%	2.49	-22.7%	[50]
N-Pentane	Dichloromethane	298.2	3.41	3.34	-2.0%	2.48	-27.2%	146
N-Pentane	Dichloromethane	348.2	2.50	2.47	-1.1%	1.74	-30.3%	146
N-Pentane	Dichloromethane	398.2	1.91	2.01	5.1%	1.31	-31.5%	146
N-Pentane	Diethyl Phthalate	303.2	4.05	4.24	4.7%	M.G.	N.A.	[39]
N-Pentane	Diethyl Phthalate	313.2	3.81	3.93	3.1%	M.G.	N.A.	[39]
N-Pentane	Diethyl Phthalate	323.2	3.67	3.66	-0.3%	M.G.	N.A.	[39]
N-Pentane	Diethyl Phthalate	333.2	3.50	3.43	-2.0%	M.G.	N.A.	[39]
N-Pentane	Dimethyl Sulfoxide	298.2	42.40	47.36	11.7%	53.53	26.3%	[50]
N-Pentane	Epsilon-Caprolactone	303.2	10.30	11.01	6.9%	M.G.	N.A.	[41]

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N-Pentane	Epsilon-Caprolactone	318.2	9.74	9.22	-5.3%	M.G.	N.A.	[41]
N-Pentane	Epsilon-Caprolactone	333.2	9.02	7.88	-12.6%	M.G.	N.A.	[41]
N-Pentane	Ethanol	293.2	9.60	9.65	0.5%	8.66	-9.8%	[10]
N-Pentane	Ethanol	298.2	7.78	9.53	22.5%	8.55	9.9%	[50]
N-Pentane	Ethanol	298.2	9.49	9.53	0.4%	8.55	-9.9%	[30]
N-Pentane	Ethanol	299.7	8.90	9.48	6.5%	8.51	-4.4%	[48]
N-Pentane	Ethanol	303.2	9.25	9.38	1.4%	8.42	-9.0%	[18]
N-Pentane	Ethanol	304.2	9.10	9.35	2.7%	8.40	-7.7%	[48]
N-Pentane	Ethanol	310.4	8.70	9.13	4.9%	8.22	-5.5%	[48]
N-Pentane	Ethanol	312.1	8.60	9.07	5.5%	8.17	-5.0%	[48]
N-Pentane	Ethanol	313.2	8.76	9.03	3.1%	8.14	-7.1%	[18]
N-Pentane	Ethanol	313.2	8.27	9.03	9.2%	8.14	-1.6%	[75]
N-Pentane	Ethanol	322.0	8.50	8.68	2.1%	7.85	-7.6%	[48]
N-Pentane	Ethanol	322.2	8.30	8.67	4.5%	7.84	-5.5%	[48]
N-Pentane	Ethanol	323.2	8.25	8.63	4.6%	7.81	-5.3%	[18]
N-Pentane	Ethanol	324.7	8.30	8.56	3.1%	7.75	-6.6%	[48]
N-Pentane	Ethanol	335.2	8.20	8.10	-1.2%	7.36	-10.2%	[48]
N-Pentane	Ethanol	343.0	7.80	7.75	-0.6%	7.04	-9.7%	[48]
N-Pentane	Ethanol	352.4	7.00	7.33	4.7%	6.64	-5.1%	[48]
N-Pentane	Ethanol	354.2	6.90	7.25	5.1%	6.56	-4.9%	[48]
N-Pentane	Ethanol	354.4	7.40	7.24	-2.2%	6.55	-11.5%	[48]
N-Pentane	Ethyl Acetate	293.2	3.09	3.00	-2.9%	2.93	-5.2%	[10]
N-Pentane	Ethyl Acetate	298.2	3.02	2.92	-3.3%	2.84	-6.0%	[50]
N-Pentane	Ethyl Acetate	303.2	2.96	2.84	-4.1%	2.75	-7.1%	[75]
N-Pentane	Ethyl Benzoate	313.2	2.77	2.77	0.0%	M.G.	N.A.	[41]
N-Pentane	Ethyl Benzoate	323.2	2.72	2.64	-2.9%	M.G.	N.A.	[41]
N-Pentane	Ethyl Benzoate	333.2	2.65	2.53	-4.5%	M.G.	N.A.	[41]
N-Pentane	Ethyl Benzoate	343.2	2.61	2.43	-6.9%	M.G.	N.A.	[41]
N-Pentane	Isopropanol	298.2	5.39	5.09	-5.6%	4.54	-15.8%	[50]
N-Pentane	Isopropanol	308.2	6.42	4.96	-22.7%	4.44	-30.8%	[47]
N-Pentane	Methanol	298.2	18.42	21.76	18.1%	17.71	-3.9%	[50]
N-Pentane	Methanol	298.2	19.50	21.76	11.6%	17.71	-9.2%	[30]
N-Pentane	Methanol	303.2	20.30	21.24	4.6%	17.31	-14.7%	[18]
N-Pentane	Methanol	313.2	18.50	20.02	8.2%	16.53	-10.6%	[18]
N-Pentane	Methyl Acetate	298.2	4.61	4.42	-4.1%	4.03	-12.6%	[50]
N-Pentane	Methyl Ethyl Ketone	293.2	3.66	3.71	1.4%	3.97	8.5%	[10]
N-Pentane	Methyl Ethyl Ketone	298.2	3.39	3.59	5.9%	3.86	13.9%	[50]
N-Pentane	Methyl Ethyl Ketone	303.2	3.76	3.47	-7.7%	3.76	0.0%	[18]
N-Pentane	Methyl Ethyl Ketone	313.2	3.56	3.27	-8.1%	3.56	0.0%	[18]
N-Pentane	Methyl Ethyl Ketone	323.2	3.43	3.09	-9.9%	3.38	-1.5%	[62]
N-Pentane	Methyl Isobutyl Ketone	293.2	2.30	2.41	4.8%	2.65	15.2%	[5]
N-Pentane	N,N-Dibutylformamide	302.8	2.48	2.81	13.2%	2.61	5.2%	[13]
N-Pentane	N,N-Dibutylformamide	318.3	2.37	2.58	9.1%	2.53	7.0%	[13]
N-Pentane	N,N-Dibutylformamide	332.4	2.27	2.41	6.1%	2.47	8.8%	[13]
N-Pentane	N,N-Diethylacetamide	303.2	4.33	4.44	2.5%	2.24	-48.3%	[39]
N-Pentane	N,N-Diethylacetamide	313.2	4.08	4.13	1.2%	2.17	-46.8%	[39]
N-Pentane	N,N-Diethylacetamide	323.2	3.94	3.86	-2.0%	2.11	-46.4%	[39]
N-Pentane	N,N-Diethylacetamide	333.2	3.74	3.63	-2.9%	2.06	-44.9%	[39]
N-Pentane	N,N-Dimethylacetamide	298.2	8.46	8.65	2.2%	7.48	-11.6%	[50]
N-Pentane	N,N-Dimethylacetamide	303.6	7.96	8.14	2.3%	7.17	-9.9%	[13]
N-Pentane	N,N-Dimethylacetamide	317.6	6.86	7.04	2.7%	6.46	-5.8%	[13]
N-Pentane	N,N-Dimethylacetamide	333.4	5.89	6.10	3.6%	5.83	-1.0%	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
N-Pentane	N,N-Dimethylformamide	298.2	11.75	13.14	11.8%	12.68	7.9%	[50]
N-Pentane	N-Decane	298.2	0.88	0.97	10.2%	0.96	9.1%	[50]
N-Pentane	N-Decane	333.2	0.94	0.97	3.2%	0.96	2.1%	[81]
N-Pentane	N-Decane	343.2	0.93	0.96	3.2%	0.96	3.2%	[81]
N-Pentane	N-Dodecane	298.2	0.88	0.95	8.0%	0.93	5.7%	[50]
N-Pentane	N-Ethylacetamide	303.2	7.55	8.34	10.5%	M.G.	N.A.	[39]
N-Pentane	N-Ethylacetamide	313.2	7.35	7.86	6.9%	M.G.	N.A.	[39]
N-Pentane	N-Ethylacetamide	323.2	7.23	7.40	2.4%	M.G.	N.A.	[39]
N-Pentane	N-Ethylacetamide	333.2	7.03	6.96	-1.0%	M.G.	N.A.	[39]
N-Pentane	N-Formylmorpholine	313.3	23.60	21.44	-9.2%	M.G.	N.A.	[43]
N-Pentane	N-Formylmorpholine	332.7	19.30	16.29	-15.6%	M.G.	N.A.	[43]
N-Pentane	N-Formylmorpholine	352.5	16.40	12.77	-22.1%	M.G.	N.A.	[43]
N-Pentane	N-Formylmorpholine	373.4	13.50	10.22	-24.3%	M.G.	N.A.	[43]
N-Pentane	N-Heptane	293.2	1.00	1.01	1.0%	1.00	0.0%	[10]
N-Pentane	N-Heptane	298.2	0.99	1.01	2.0%	1.00	1.0%	[50]
N-Pentane	N-Hexadecane	298.2	0.84	0.86	2.4%	0.87	3.6%	[50]
N-Pentane	N-Hexadecane	298.2	0.87	0.86	-1.6%	0.87	-0.5%	[6]
N-Pentane	N-Hexane	298.2	0.99	1.01	2.0%	1.00	1.0%	[50]
N-Pentane	Nitrobenzene	293.2	7.46	6.75	-9.5%	6.98	-6.4%	[10]
N-Pentane	Nitrobenzene	298.2	6.56	6.41	-2.3%	6.79	3.5%	[50]
N-Pentane	Nitroethane	293.2	9.62	10.33	7.4%	7.34	-23.7%	[10]
N-Pentane	Nitromethane	298.2	31.47	27.77	-11.8%	34.05	8.2%	[50]
N-Pentane	N-Methyl-2-Pyrrolidone	298.2	9.60	12.40	29.2%	8.25	-14.1%	[50]
N-Pentane	N-Methyl-2-Pyrrolidone	323.4	11.50	9.32	-19.0%	7.52	-34.6%	[43]
N-Pentane	N-Methyl-2-Pyrrolidone	333.2	10.20	8.47	-17.0%	7.20	-29.4%	[43]
N-Pentane	N-Methyl-2-Pyrrolidone	343.4	9.35	7.73	-17.3%	6.87	-26.5%	[43]
N-Pentane	N-Methylacetamide	303.4	11.96	13.06	9.2%	12.31	2.9%	[13]
N-Pentane	N-Methylacetamide	318.4	11.37	11.77	3.5%	11.77	3.5%	[13]
N-Pentane	N-Methylacetamide	333.2	10.85	10.58	-2.5%	11.28	4.0%	[13]
N-Pentane	N-Methylformamide	298.2	22.84	30.87	35.2%	M.P.	N.A.	[50]
N-Pentane	N-Methylformamide	303.2	31.51	29.24	-7.2%	M.P.	N.A.	[35]
N-Pentane	N-Methylformamide	313.2	28.60	26.20	-8.4%	M.P.	N.A.	[35]
N-Pentane	N-Methylformamide	323.2	26.40	23.45	-11.2%	M.P.	N.A.	[35]
N-Pentane	N-Methylformamide	333.2	24.49	21.00	-14.3%	M.P.	N.A.	[35]
N-Pentane	N-Nonane	298.2	0.95	0.99	4.2%	0.98	3.2%	[50]
N-Pentane	N-Nonane	333.2	0.96	0.98	2.1%	0.98	2.1%	[81]
N-Pentane	N-Octane	293.2	1.01	1.00	-1.0%	0.99	-2.0%	[74]
N-Pentane	N-Octane	293.2	0.97	1.00	3.1%	0.99	2.1%	[10]
N-Pentane	N-Octane	298.2	0.98	1.00	2.0%	0.99	1.0%	[50]
N-Pentane	N-Octane	313.2	1.00	1.00	0.0%	0.99	-1.0%	[36]
N-Pentane	N-Octane	333.2	0.98	0.99	1.0%	0.99	1.0%	[81]
N-Pentane	N-Octane	333.2	1.05	0.99	-5.7%	0.99	-5.7%	[36]
N-Pentane	N-Pentane	298.2	1.05	1.00	-4.8%	1.00	-4.8%	[50]
N-Pentane	Phenol	323.2	10.90	11.21	2.8%	9.93	-8.9%	[10]
N-Pentane	Propionitrile	293.2	8.53	10.21	19.7%	8.36	-2.0%	[10]
N-Pentane	Propionitrile	298.2	7.76	9.53	22.8%	8.06	3.9%	[50]
N-Pentane	P-Xylene	293.2	1.48	1.53	3.4%	1.61	8.8%	[10]
N-Pentane	P-Xylene	298.2	1.46	1.51	3.4%	1.60	9.6%	[50]
N-Pentane	Pyridine	298.2	5.40	5.70	5.6%	6.98	29.3%	[50]
N-Pentane	Quinoline	293.2	7.81	6.93	-11.3%	M.G.	N.A.	[37]
N-Pentane	Squalane	298.2	0.58	0.51	-12.1%	0.68	17.2%	[50]
N-Pentane	Sulfolane	303.4	34.63	36.21	4.6%	M.G.	N.A.	[13]

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N-Pentane	Sulfolane	317.9	30.44	27.40	-10.0%	M.G.	N.A.	[13]
N-Pentane	Sulfolane	332.6	27.26	21.37	-21.6%	M.G.	N.A.	[13]
N-Pentane	Tetraethylene Glycol DME	303.2	3.48	3.55	2.2%	1.79	-48.5%	[7]
N-Pentane	Tetraethylene Glycol DME	323.2	3.10	3.13	1.0%	1.67	-46.1%	[7]
N-Pentane	Tetraethylene Glycol DME	343.2	2.78	2.81	1.1%	1.57	-43.5%	[7]
N-Pentane	Tetrahydrofuran	298.2	2.07	2.17	4.8%	1.91	-7.7%	[50]
N-Pentane	Tetrahydrofuran	313.2	2.04	2.04	0.0%	1.81	-11.3%	[19]
N-Pentane	Toluene	293.2	1.85	1.94	4.9%	1.80	-2.7%	[33]
N-Pentane	Toluene	293.2	1.83	1.94	6.0%	1.80	-1.6%	[33]
N-Pentane	Toluene	293.2	1.64	1.94	18.3%	1.80	9.8%	[30]
N-Pentane	Toluene	293.2	1.80	1.94	7.8%	1.80	0.0%	[10]
N-Pentane	Toluene	298.2	1.68	1.91	13.7%	1.78	6.0%	[50]
N-Pentane	Toluene	303.2	1.78	1.88	5.6%	1.77	-0.6%	[33]
N-Pentane	Toluene	303.2	1.61	1.88	16.8%	1.77	9.9%	[30]
N-Pentane	Toluene	313.2	1.95	1.82	-6.7%	1.73	-11.3%	[33]
N-Pentane	Toluene	313.2	1.58	1.82	15.2%	1.73	9.5%	[30]
N-Pentane	Tributyl Phosphate	298.6	1.73	1.63	-5.8%	M.G.	N.A.	[27]
N-Pentane	Tributyl Phosphate	302.9	1.88	1.60	-14.9%	M.G.	N.A.	[27]
N-Pentane	Tributyl Phosphate	308.6	1.75	1.56	-10.9%	M.G.	N.A.	[27]
N-Pentane	Tributyl Phosphate	313.1	1.62	1.53	-5.6%	M.G.	N.A.	[27]
N-Pentane	Tributyl Phosphate	323.7	1.57	1.47	-6.4%	M.G.	N.A.	[27]
N-Pentane	Tributyl Phosphate	330.0	1.46	1.44	-1.4%	M.G.	N.A.	[27]
N-Pentane	Triethylamine	298.2	1.03	1.03	0.0%	1.04	1.0%	[50]
Phenol	Benzene	353.2	3.30	5.03	52.4%	2.88	-12.7%	582
Phenol	Ethyl Acetate	300.0	0.31	0.33	5.5%	0.15	-52.0%	396
Phenol	Ethyl Acetate	320.0	0.47	0.40	-14.1%	0.18	-61.3%	396
Phenol	Ethylene Glycol Ethyl Ether	363.2	0.17	0.13	-22.1%	0.20	19.8%	398
Phenol	Ethylene Glycol Ethyl Ether	373.2	0.19	0.14	-26.8%	0.20	4.6%	398
Phenol	Ethylene Glycol Ethyl Ether	383.2	0.21	0.15	-28.8%	0.20	-5.0%	398
Phenol	N-Decane	418.2	6.33	8.54	35.0%	5.23	-17.3%	44
Phenol	N-Decane	433.2	4.79	7.03	46.7%	4.51	-5.9%	44
Phenol	N-Methylacetamide	413.5	0.10	0.07	-30.0%	M.P.	N.A.	327
Propane	Benzyl Alcohol	298.2	8.02	5.57	-30.5%	5.89	-26.6%	[67]
Propionitrile	1-Butanol	293.2	5.20	5.61	7.9%	3.19	-38.7%	[10]
Propionitrile	1-Octanol	293.2	6.34	6.46	1.9%	3.23	-49.1%	[10]
Propionitrile	1-Octanol	298.2	5.46	6.12	12.1%	3.09	-43.4%	[3]
Propionitrile	2,2,4-Trimethylpentane	293.2	20.00	17.95	-10.3%	10.08	-49.6%	[10]
Propionitrile	Carbon Tetrachloride	293.2	7.20	6.57	-8.8%	4.63	-35.7%	[10]
Propionitrile	Ethyl Acetate	311.6	1.42	1.33	-6.3%	1.29	-9.2%	[12]
Propionitrile	Ethyl Acetate	329.2	1.35	1.29	-4.4%	1.31	-3.0%	[12]
Propionitrile	Ethyl Acetate	348.2	1.29	1.26	-2.3%	1.32	2.3%	[12]
Propionitrile	Ethylbenzene	313.2	2.64	2.88	9.0%	2.22	-16.0%	312
Propionitrile	Ethylbenzene	353.2	2.42	2.32	-4.2%	2.14	-11.7%	312
Propionitrile	Ethylbenzene	393.2	2.23	1.97	-11.5%	2.07	-7.0%	312
Propionitrile	N-Heptane	293.2	21.90	18.24	-16.7%	11.01	-49.7%	[10]
Propionitrile	N-Heptane	313.2	16.54	12.83	-22.4%	8.89	-46.3%	125
Propionitrile	N-Hexadecane	298.2	15.58	13.30	-14.6%	6.19	-60.3%	[6]
Propionitrile	N-Hexane	295.0	19.20	18.14	-5.5%	11.99	-37.6%	[12]
Propionitrile	N-Hexane	313.2	14.64	13.22	-9.7%	9.88	-32.5%	126
Propionitrile	N-Hexane	322.9	13.60	11.40	-16.2%	8.97	-34.0%	[12]
Propionitrile	N-Hexane	332.3	10.70	10.00	-6.5%	8.21	-23.3%	[12]
Propionitrile	N-Hexane	340.9	10.00	8.94	-10.6%	7.60	-24.0%	[12]

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Propionitrile	N-Octane	293.2	20.90	17.74	-15.1%	10.09	-51.7%	[10]
Propionitrile	N-Octane	313.2	15.43	12.46	-19.2%	8.15	-47.2%	124
Propionitrile	Toluene	293.2	2.64	2.93	11.0%	1.89	-28.4%	[10]
Propionitrile	Tributyl Phosphate	298.6	0.86	0.91	5.8%	M.G.	N.A.	[27]
Propionitrile	Tributyl Phosphate	302.9	0.89	0.90	1.1%	M.G.	N.A.	[27]
Propionitrile	Tributyl Phosphate	308.6	0.87	0.89	2.3%	M.G.	N.A.	[27]
Propionitrile	Tributyl Phosphate	313.1	0.90	0.88	-2.2%	M.G.	N.A.	[27]
Propionitrile	Tributyl Phosphate	323.7	0.85	0.87	2.4%	M.G.	N.A.	[27]
Propionitrile	Tributyl Phosphate	330.0	0.80	0.86	7.5%	M.G.	N.A.	[27]
Propyl Acetate	1-Octanol	298.2	2.36	2.46	4.2%	1.59	-32.6%	[3]
Propyl Acetate	1-Pentanol	303.5	3.17	2.49	-21.5%	1.60	-49.5%	[33]
Propyl Acetate	1-Pentanol	313.2	2.78	2.41	-13.3%	1.48	-46.8%	[33]
Propyl Acetate	1-Pentanol	323.5	2.20	2.32	5.5%	1.37	-37.7%	[33]
Propyl Acetate	Ethylene Glycol Ethyl Ether	313.2	2.05	1.85	-9.9%	1.02	-50.3%	391
Propyl Acetate	N,N-Dibutylformamide	302.8	1.38	1.19	-13.5%	1.09	-20.7%	[13]
Propyl Acetate	N,N-Dibutylformamide	318.3	1.29	1.17	-9.3%	1.06	-17.8%	[13]
Propyl Acetate	N,N-Dibutylformamide	332.5	1.26	1.16	-7.7%	1.04	-17.3%	[13]
Propyl Acetate	N,N-Dimethylacetamide	303.3	2.01	1.66	-17.5%	0.91	-54.8%	[13]
Propyl Acetate	N,N-Dimethylacetamide	317.6	1.87	1.60	-14.6%	0.88	-53.0%	[13]
Propyl Acetate	N,N-Dimethylacetamide	333.0	1.75	1.55	-11.3%	0.83	-52.5%	[13]
Propyl Acetate	N-Formylmorpholine	303.5	3.18	3.37	6.0%	M.G.	N.A.	[43]
Propyl Acetate	N-Formylmorpholine	323.2	2.97	3.03	2.0%	M.G.	N.A.	[43]
Propyl Acetate	N-Formylmorpholine	342.8	2.84	2.76	-2.8%	M.G.	N.A.	[43]
Propyl Acetate	N-Hexadecane	298.2	2.60	3.80	46.4%	2.98	14.8%	[6]
Propyl Acetate	N-Methyl-2-Pyrrolidone	323.4	2.16	2.40	11.1%	M.P.	N.A.	[43]
Propyl Acetate	N-Methyl-2-Pyrrolidone	333.2	2.14	2.32	8.4%	M.P.	N.A.	[43]
Propyl Acetate	N-Methyl-2-Pyrrolidone	343.4	2.12	2.25	6.1%	M.P.	N.A.	[43]
Propyl Acetate	N-Methylacetamide	304.2	3.29	3.49	6.2%	1.52	-53.7%	[13]
Propyl Acetate	N-Methylacetamide	318.4	3.18	3.36	5.7%	1.50	-52.8%	[13]
Propyl Acetate	N-Methylacetamide	333.2	3.05	3.21	5.4%	1.47	-51.7%	[13]
Propyl Acetate	Sulfolane	303.1	3.66	3.90	6.5%	M.G.	N.A.	[13]
Propyl Acetate	Sulfolane	317.9	3.50	3.52	0.5%	M.G.	N.A.	[13]
Propyl Acetate	Sulfolane	332.6	3.37	3.22	-4.3%	M.G.	N.A.	[13]
Propyl Acetate	Tetraethylene Glycol DME	303.2	0.98	1.12	14.9%	0.76	-22.1%	[7]
Propyl Acetate	Tetraethylene Glycol DME	323.2	0.96	1.10	14.7%	0.78	-18.7%	[7]
Propyl Acetate	Tributyl Phosphate	298.6	0.97	0.75	-22.7%	M.G.	N.A.	[27]
Propyl Acetate	Tributyl Phosphate	302.9	0.97	0.75	-22.7%	M.G.	N.A.	[27]
Propyl Acetate	Tributyl Phosphate	308.6	0.97	0.75	-22.7%	M.G.	N.A.	[27]
Propyl Acetate	Tributyl Phosphate	313.1	0.99	0.75	-24.2%	M.G.	N.A.	[27]
P-Xylene	1-Butanol	313.2	4.22	3.34	-20.9%	3.34	-20.9%	62
P-Xylene	1-Octanol	303.5	2.11	2.13	0.9%	1.93	-8.5%	[31]
P-Xylene	1-Octanol	313.6	2.00	2.07	3.5%	1.87	-6.5%	[31]
P-Xylene	1-Octanol	323.4	1.96	2.01	2.6%	1.81	-7.7%	[31]
P-Xylene	1-Propanol	313.2	5.34	4.28	-19.9%	4.38	-18.0%	61
P-Xylene	2,2,4-Trimethylpentane	313.2	1.48	1.55	4.8%	1.43	-3.3%	97
P-Xylene	2-Methyl-1-Propanol	313.2	4.72	3.45	-26.9%	3.34	-29.2%	21
P-Xylene	2-Methyl-2-Propanol	313.2	3.71	2.76	-25.6%	3.73	0.5%	18
P-Xylene	2-Pyrrolidone	303.2	6.07	6.90	13.6%	M.G.	N.A.	[35]
P-Xylene	2-Pyrrolidone	313.2	6.01	6.29	4.7%	M.G.	N.A.	[35]
P-Xylene	2-Pyrrolidone	323.2	5.93	5.77	-2.7%	M.G.	N.A.	[35]
P-Xylene	2-Pyrrolidone	333.2	5.87	5.31	-9.5%	M.G.	N.A.	[35]
P-Xylene	Benzene	308.2	1.07	1.02	-4.6%	1.01	-5.5%	133

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
P-Xylene	Ethanol	313.2	7.11	6.48	-8.8%	6.67	-6.1%	96
P-Xylene	Ethyl Benzoate	313.2	1.10	1.16	5.5%	M.G.	N.A.	[41]
P-Xylene	Ethyl Benzoate	323.2	1.11	1.15	3.6%	M.G.	N.A.	[41]
P-Xylene	Ethyl Benzoate	333.2	1.12	1.14	1.8%	M.G.	N.A.	[41]
P-Xylene	Ethyl Benzoate	343.2	1.13	1.14	0.9%	M.G.	N.A.	[41]
P-Xylene	Methanol	313.2	12.76	11.44	-10.4%	12.88	0.9%	46
P-Xylene	N-Decane	313.2	1.23	1.24	0.9%	1.28	4.1%	100
P-Xylene	N-Formylmorpholine	313.3	4.07	5.27	29.5%	M.G.	N.A.	[43]
P-Xylene	N-Formylmorpholine	332.7	3.84	4.53	18.0%	M.G.	N.A.	[43]
P-Xylene	N-Formylmorpholine	352.5	3.71	3.96	6.7%	M.G.	N.A.	[43]
P-Xylene	N-Formylmorpholine	373.4	3.56	3.49	-2.0%	M.G.	N.A.	[43]
P-Xylene	N-Heptane	313.2	1.38	1.37	-0.9%	1.53	10.7%	102
P-Xylene	N-Hexadecane	453.2	0.83	0.90	8.4%	0.83	0.0%	[71]
P-Xylene	N-Hexane	313.2	1.47	1.42	-3.6%	1.67	13.4%	103
P-Xylene	N-Methyl-2-Pyrrolidone	373.2	1.69	1.81	7.1%	1.42	-15.9%	323
P-Xylene	N-Methyl-2-Pyrrolidone	473.2	1.57	1.53	-2.7%	1.29	-18.0%	323
P-Xylene	N-Methylformamide	303.2	10.59	9.87	-6.8%	M.P.	N.A.	[35]
P-Xylene	N-Methylformamide	313.2	10.33	9.21	-10.8%	M.P.	N.A.	[35]
P-Xylene	N-Methylformamide	323.2	10.06	8.56	-14.9%	M.P.	N.A.	[35]
P-Xylene	N-Methylformamide	333.2	9.81	7.95	-19.0%	M.P.	N.A.	[35]
P-Xylene	N-Octane	313.2	1.31	1.32	1.1%	1.43	9.6%	101
P-Xylene	Phenol	343.2	3.49	3.27	-6.3%	2.66	-23.8%	[14]
P-Xylene	Phenol	358.2	3.26	3.12	-4.3%	2.51	-23.0%	[14]
P-Xylene	Phenol	373.2	3.22	2.96	-8.1%	2.37	-26.4%	[14]
P-Xylene	Tetraethylene Glycol DME	303.2	1.18	1.19	0.6%	1.04	-12.1%	[7]
P-Xylene	Tetraethylene Glycol DME	323.2	1.10	1.16	5.6%	1.03	-6.3%	[7]
P-Xylene	Tetraethylene Glycol DME	343.2	1.07	1.14	7.0%	1.01	-5.2%	[7]
P-Xylene	Tributyl Phosphate	298.6	0.84	0.76	-9.5%	M.G.	N.A.	[27]
P-Xylene	Tributyl Phosphate	302.9	0.84	0.76	-9.5%	M.G.	N.A.	[27]
P-Xylene	Tributyl Phosphate	308.6	0.84	0.76	-9.5%	M.G.	N.A.	[27]
P-Xylene	Tributyl Phosphate	313.1	0.84	0.76	-9.5%	M.G.	N.A.	[27]
P-Xylene	Tributyl Phosphate	333.2	0.86	0.76	-11.6%	M.G.	N.A.	[73]
P-Xylene	Tributyl Phosphate	363.2	0.86	0.76	-11.6%	M.G.	N.A.	[20]
P-Xylene	Tributyl Phosphate	373.2	0.89	0.76	-14.6%	M.G.	N.A.	[20]
P-Xylene	Tributyl Phosphate	383.2	0.87	0.76	-12.6%	M.G.	N.A.	[20]
Pyridine	1,2-Dichloroethane	330.0	0.90	0.82	-8.9%	0.26	-71.1%	[12]
Pyridine	1,2-Dichloroethane	354.3	0.89	0.84	-5.6%	0.24	-73.0%	[12]
Pyridine	1-Butanol	313.2	0.84	1.17	39.9%	0.66	-21.1%	182
Pyridine	1-Chlorobutane	349.3	1.38	1.73	25.4%	1.06	-23.2%	[12]
Pyridine	1-Octanol	298.2	0.72	1.30	80.8%	0.45	-37.4%	[3]
Pyridine	1-Phenyl-1-Butanone	298.1	0.92	1.09	18.5%	0.83	-9.8%	[34]
Pyridine	1-Propanol	313.2	0.83	1.02	22.8%	0.80	-3.7%	184
Pyridine	2,2,4-Trimethylpentane	293.2	5.91	6.32	7.0%	4.73	-19.9%	158
Pyridine	2,2,4-Trimethylpentane	298.2	5.62	5.90	5.0%	4.46	-20.6%	158
Pyridine	2,2,4-Trimethylpentane	303.2	5.43	5.53	1.9%	4.22	-22.2%	158
Pyridine	2,2,4-Trimethylpentane	308.2	5.19	5.20	0.2%	4.01	-22.7%	158
Pyridine	2,2,4-Trimethylpentane	313.2	4.95	4.91	-0.8%	3.84	-22.4%	158
Pyridine	2-Butanol	313.2	0.83	1.23	48.6%	0.66	-20.3%	181
Pyridine	2-Methyl-1-Propanol	313.2	0.77	1.22	58.8%	0.66	-14.1%	180
Pyridine	2-Methyl-2-Propanol	313.2	0.87	1.25	43.7%	1.14	31.1%	179
Pyridine	Acetone	303.2	1.30	1.51	15.9%	1.31	0.5%	297
Pyridine	Acetonitrile	315.8	1.92	1.39	-27.6%	1.69	-12.0%	[12]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Pyridine	Acetonitrile	334.6	1.81	1.35	-25.4%	1.67	-7.7%	[12]
Pyridine	Acetonitrile	352.6	1.75	1.32	-24.6%	1.65	-5.7%	[12]
Pyridine	Benzene	298.2	1.25	1.58	26.6%	1.34	7.3%	82
Pyridine	Benzene	303.2	1.25	1.55	24.5%	1.34	7.6%	82
Pyridine	Benzene	313.2	1.25	1.50	20.2%	1.34	7.3%	82
Pyridine	Benzene	323.2	1.25	1.46	16.6%	1.34	7.0%	82
Pyridine	Benzene	329.7	1.21	1.43	18.2%	1.34	10.7%	[12]
Pyridine	Benzene	351.1	1.22	1.36	11.5%	1.32	8.2%	[12]
Pyridine	Chloroform	303.2	0.29	0.20	-31.0%	0.63	117.4%	293
Pyridine	Cyclohexane	293.2	6.24	5.95	-4.6%	6.04	-3.2%	157
Pyridine	Cyclohexane	298.2	5.96	5.58	-6.4%	5.54	-7.1%	157
Pyridine	Cyclohexane	303.2	5.55	5.25	-5.5%	5.10	-8.2%	157
Pyridine	Cyclohexane	308.2	5.27	4.95	-6.0%	4.72	-10.4%	157
Pyridine	Cyclohexane	313.2	5.00	4.68	-6.5%	4.38	-12.5%	157
Pyridine	Dichloromethane	303.2	0.58	0.46	-21.3%	0.62	6.0%	296
Pyridine	Ethanol	313.2	0.96	1.14	18.2%	1.08	12.0%	185
Pyridine	Ethanol	336.4	0.96	1.12	16.7%	1.14	18.8%	[12]
Pyridine	Ethanol	350.6	0.94	1.11	18.1%	1.22	29.8%	[12]
Pyridine	Isopropanol	313.2	0.99	1.32	33.6%	0.92	-6.9%	183
Pyridine	Methanol	298.2	0.82	0.95	15.7%	0.81	-1.3%	257
Pyridine	Methanol	308.2	0.87	0.94	8.0%	0.86	-1.2%	257
Pyridine	Methanol	313.2	0.89	0.94	5.3%	0.88	-1.4%	257
Pyridine	Methanol	318.2	0.91	0.93	2.0%	0.91	-0.2%	257
Pyridine	Methyl Ethyl Ketone	342.3	1.13	1.24	9.7%	1.10	-2.7%	[10]
Pyridine	N,N-Dibutylformamide	302.8	0.63	0.89	40.4%	M.P.	N.A.	[13]
Pyridine	N,N-Dibutylformamide	318.3	0.74	0.88	18.4%	M.P.	N.A.	[13]
Pyridine	N,N-Dibutylformamide	332.5	0.78	0.87	11.0%	M.P.	N.A.	[13]
Pyridine	N,N-Dimethylacetamide	303.4	0.64	0.97	52.0%	M.P.	N.A.	[13]
Pyridine	N,N-Dimethylacetamide	317.6	0.82	0.97	18.0%	M.P.	N.A.	[13]
Pyridine	N,N-Dimethylacetamide	333.0	1.05	0.98	-6.5%	M.P.	N.A.	[13]
Pyridine	N-Heptane	298.2	5.56	5.40	-2.8%	5.04	-9.3%	588
Pyridine	N-Heptane	303.1	5.21	5.08	-2.4%	4.77	-8.4%	588
Pyridine	N-Heptane	313.2	4.80	4.52	-5.7%	4.34	-9.5%	588
Pyridine	N-Heptane	313.2	4.62	4.52	-2.2%	4.34	-6.1%	588
Pyridine	N-Heptane	323.2	4.20	4.07	-3.0%	4.02	-4.2%	588
Pyridine	N-Heptane	333.2	3.82	3.71	-2.9%	3.78	-1.1%	588
Pyridine	N-Heptane	341.0	3.81	3.46	-9.1%	3.64	-4.4%	588
Pyridine	N-Heptane	353.2	3.36	3.14	-6.5%	3.47	3.3%	588
Pyridine	N-Hexadecane	298.2	3.39	3.83	13.1%	2.58	-23.8%	[6]
Pyridine	N-Hexane	296.6	5.90	5.85	-0.8%	5.98	1.4%	[12]
Pyridine	N-Hexane	298.2	6.23	5.73	-8.0%	5.87	-5.8%	59
Pyridine	N-Hexane	303.2	5.85	5.38	-8.1%	5.55	-5.2%	59
Pyridine	N-Hexane	313.2	5.18	4.79	-7.5%	5.05	-2.5%	59
Pyridine	N-Hexane	316.9	4.83	4.61	-4.6%	4.90	1.4%	[12]
Pyridine	N-Hexane	323.2	4.64	4.32	-6.8%	4.68	0.9%	59
Pyridine	N-Hexane	328.2	4.40	4.11	-6.5%	4.53	3.0%	59
Pyridine	N-Hexane	330.1	4.22	4.04	-4.3%	4.48	6.2%	[12]
Pyridine	N-Hexane	340.4	4.04	3.69	-8.7%	4.24	5.0%	[12]
Pyridine	N-Methylacetamide	318.4	1.53	1.32	-13.4%	1.60	4.9%	[13]
Pyridine	N-Methylacetamide	331.9	1.58	1.31	-17.2%	1.59	0.5%	[13]
Pyridine	N-Methylacetamide	398.6	1.53	1.25	-18.3%	1.57	2.6%	328
Pyridine	N-Octane	313.2	4.34	4.31	-0.7%	3.85	-11.3%	588

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Pyridine	N-Octane	353.2	3.04	2.99	-1.6%	3.07	1.0%	588
Pyridine	N-Octane	369.8	2.58	2.67	3.5%	2.94	14.0%	588
Pyridine	Propionitrile	323.3	1.36	1.31	-3.7%	1.26	-7.4%	[12]
Pyridine	Propionitrile	338.0	1.39	1.29	-7.2%	1.24	-10.8%	[12]
Pyridine	Sulfolane	317.9	1.17	1.47	25.2%	M.G.	N.A.	[13]
Pyridine	Sulfolane	332.7	1.05	1.43	36.5%	M.G.	N.A.	[13]
Pyridine	Tetraethylene Glycol DME	303.2	0.52	0.82	56.5%	0.37	-29.4%	[7]
Pyridine	Tetraethylene Glycol DME	323.2	0.54	0.81	51.1%	0.50	-6.7%	[7]
Pyridine	Tetraethylene Glycol DME	343.2	0.57	0.80	40.6%	0.68	19.5%	[7]
Pyridine	Toluene	293.2	1.67	1.77	5.9%	1.47	-12.0%	238
Pyridine	Toluene	298.2	1.91	1.73	-9.3%	1.46	-23.5%	238
Pyridine	Toluene	298.2	1.62	1.73	6.9%	1.46	-9.8%	238
Pyridine	Toluene	303.2	1.76	1.69	-4.0%	1.46	-17.0%	238
Pyridine	Toluene	303.2	1.59	1.69	6.1%	1.46	-8.4%	238
Pyridine	Toluene	308.2	1.59	1.66	4.5%	1.45	-8.7%	238
Pyridine	Toluene	313.2	1.55	1.63	5.1%	1.45	-6.5%	238
Pyridine	Toluene	313.2	1.60	1.63	2.0%	1.45	-9.2%	238
Pyridine	Toluene	323.2	1.48	1.57	5.9%	1.44	-2.9%	238
Pyridine	Toluene	333.2	1.45	1.52	4.9%	1.43	-1.3%	238
Pyridine	Toluene	373.2	1.34	1.37	2.0%	1.39	3.5%	238
Tetrahydrofuran	1,2-Dichloroethane	303.2	0.62	0.67	8.1%	0.55	-11.3%	[15]
Tetrahydrofuran	1,2-Dichloroethane	323.2	0.69	0.71	2.9%	0.59	-14.5%	[15]
Tetrahydrofuran	1,2-Dichloroethane	343.2	0.72	0.75	4.2%	0.61	-15.3%	[15]
Tetrahydrofuran	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.35	1.30	-3.7%	M.G.	N.A.	[29]
Tetrahydrofuran	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.38	1.28	-7.2%	M.G.	N.A.	[29]
Tetrahydrofuran	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.40	1.26	-10.0%	M.G.	N.A.	[29]
Tetrahydrofuran	1-Ethylpyrrolidin-2-One	298.2	1.29	1.30	0.8%	M.P.	N.A.	[29]
Tetrahydrofuran	1-Ethylpyrrolidin-2-One	308.2	1.33	1.28	-3.8%	M.P.	N.A.	[29]
Tetrahydrofuran	1-Ethylpyrrolidin-2-One	318.2	1.38	1.26	-8.7%	M.P.	N.A.	[29]
Tetrahydrofuran	1-Octanol	298.2	1.01	1.09	7.9%	1.32	30.7%	[3]
Tetrahydrofuran	1-Phenyl-1-Butanone	298.1	0.81	0.84	3.7%	0.93	14.8%	[34]
Tetrahydrofuran	2,2,4-Trimethylpentane	293.2	1.36	1.79	31.6%	1.46	7.4%	[10]
Tetrahydrofuran	Carbon Tetrachloride	303.2	0.82	0.86	4.9%	0.93	13.4%	300
Tetrahydrofuran	Chloroform	303.2	0.18	0.20	11.4%	0.26	44.8%	298
Tetrahydrofuran	Chloroform	305.0	0.21	0.20	-4.8%	0.27	28.6%	[12]
Tetrahydrofuran	Chloroform	313.2	0.21	0.22	4.8%	0.28	33.3%	[15]
Tetrahydrofuran	Chloroform	313.6	0.23	0.22	-4.3%	0.28	21.7%	[60]
Tetrahydrofuran	Chloroform	323.0	0.25	0.25	0.0%	0.30	20.0%	[12]
Tetrahydrofuran	Chloroform	323.2	0.24	0.25	4.2%	0.30	25.0%	[15]
Tetrahydrofuran	Chloroform	323.4	0.26	0.25	-3.8%	0.30	15.4%	[60]
Tetrahydrofuran	Cyclohexane	298.2	2.00	1.88	-6.0%	1.75	-12.5%	307
Tetrahydrofuran	Cyclohexane	313.2	1.72	1.78	3.5%	1.65	-4.1%	[19]
Tetrahydrofuran	Cyclohexane	333.2	1.63	1.67	2.5%	1.54	-5.5%	[19]
Tetrahydrofuran	Dichloromethane	303.2	0.42	0.43	3.3%	0.70	68.2%	299
Tetrahydrofuran	Diethyl Phthalate	303.2	0.78	0.79	1.5%	M.G.	N.A.	[39]
Tetrahydrofuran	Diethyl Phthalate	313.2	0.79	0.79	0.5%	M.G.	N.A.	[39]
Tetrahydrofuran	Diethyl Phthalate	323.2	0.80	0.79	-1.1%	M.G.	N.A.	[39]
Tetrahydrofuran	Diethyl Phthalate	333.2	0.81	0.79	-2.0%	M.G.	N.A.	[39]
Tetrahydrofuran	Epsilon-Caprolactone	303.2	1.42	1.55	9.2%	M.G.	N.A.	[41]
Tetrahydrofuran	Epsilon-Caprolactone	318.2	1.41	1.50	6.4%	M.G.	N.A.	[41]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Tetrahydrofuran	Epsilon-Caprolactone	333.2	1.40	1.45	3.6%	M.G.	N.A.	[41]
Tetrahydrofuran	Ethyl Acetate	313.0	1.10	1.08	-1.8%	1.16	5.5%	[12]
Tetrahydrofuran	Ethyl Acetate	313.2	1.09	1.08	-0.9%	1.16	6.4%	[19]
Tetrahydrofuran	Ethyl Acetate	333.2	1.10	1.07	-2.7%	1.15	4.5%	[19]
Tetrahydrofuran	Ethyl Acetate	333.5	1.06	1.07	0.9%	1.15	8.5%	[12]
Tetrahydrofuran	Ethyl Acetate	348.3	1.03	1.07	3.9%	1.15	11.7%	[12]
Tetrahydrofuran	Glutaronitrile	303.2	2.09	2.46	17.7%	M.G.	N.A.	[39]
Tetrahydrofuran	Glutaronitrile	313.2	2.09	2.34	12.0%	M.G.	N.A.	[39]
Tetrahydrofuran	Glutaronitrile	323.2	2.09	2.24	7.2%	M.G.	N.A.	[39]
Tetrahydrofuran	Glutaronitrile	333.2	2.08	2.15	3.4%	M.G.	N.A.	[39]
Tetrahydrofuran	N,N-Dibutylformamide	302.8	0.88	0.84	-4.2%	1.04	18.6%	[13]
Tetrahydrofuran	N,N-Dibutylformamide	318.3	0.87	0.83	-5.0%	1.03	17.8%	[13]
Tetrahydrofuran	N,N-Dibutylformamide	332.4	0.87	0.83	-4.8%	1.01	15.8%	[13]
Tetrahydrofuran	N,N-Diethylacetamide	303.2	1.11	1.09	-1.8%	M.P.	N.A.	[39]
Tetrahydrofuran	N,N-Diethylacetamide	313.2	1.11	1.08	-2.7%	M.P.	N.A.	[39]
Tetrahydrofuran	N,N-Diethylacetamide	323.2	1.12	1.07	-4.5%	M.P.	N.A.	[39]
Tetrahydrofuran	N,N-Diethylacetamide	333.2	1.12	1.07	-4.5%	M.P.	N.A.	[39]
Tetrahydrofuran	N,N-Dimethylacetamide	303.3	1.53	1.49	-2.6%	M.P.	N.A.	[13]
Tetrahydrofuran	N,N-Dimethylacetamide	317.6	1.50	1.45	-3.1%	M.P.	N.A.	[13]
Tetrahydrofuran	N,N-Dimethylacetamide	333.6	1.46	1.41	-3.6%	M.P.	N.A.	[13]
Tetrahydrofuran	N-Ethylacetamide	303.2	1.73	1.63	-5.8%	M.G.	N.A.	[39]
Tetrahydrofuran	N-Ethylacetamide	313.2	1.71	1.62	-5.3%	M.G.	N.A.	[39]
Tetrahydrofuran	N-Ethylacetamide	323.2	1.71	1.60	-6.4%	M.G.	N.A.	[39]
Tetrahydrofuran	N-Ethylacetamide	333.2	1.70	1.58	-7.1%	M.G.	N.A.	[39]
Tetrahydrofuran	N-Heptane	303.2	1.55	1.66	7.1%	1.49	-3.9%	[15]
Tetrahydrofuran	N-Heptane	313.2	1.79	1.60	-10.6%	1.44	-19.6%	[19]
Tetrahydrofuran	N-Heptane	333.2	1.43	1.51	5.6%	1.36	-4.9%	[19]
Tetrahydrofuran	N-Heptane	343.2	1.40	1.46	4.3%	1.32	-5.7%	[15]
Tetrahydrofuran	N-Hexadecane	298.2	1.20	1.18	-1.7%	1.06	-11.7%	[6]
Tetrahydrofuran	N-Hexane	304.8	1.65	1.74	5.5%	1.58	-4.2%	[12]
Tetrahydrofuran	N-Hexane	313.2	1.73	1.69	-2.3%	1.54	-11.0%	[19]
Tetrahydrofuran	N-Hexane	322.4	1.59	1.64	3.1%	1.50	-5.7%	[12]
Tetrahydrofuran	N-Hexane	333.2	1.58	1.59	0.6%	1.45	-8.2%	[19]
Tetrahydrofuran	N-Hexane	340.2	1.51	1.56	3.3%	1.43	-5.3%	[12]
Tetrahydrofuran	N-Methylacetamide	303.1	2.13	1.97	-7.3%	M.P.	N.A.	[13]
Tetrahydrofuran	N-Methylacetamide	318.4	2.09	1.93	-7.6%	M.P.	N.A.	[13]
Tetrahydrofuran	N-Methylacetamide	333.1	2.06	1.89	-8.1%	M.P.	N.A.	[13]
Tetrahydrofuran	N-Octane	293.2	1.50	1.64	9.3%	1.46	-2.7%	[10]
Tetrahydrofuran	N-Pentane	313.2	2.19	1.81	-17.4%	1.68	-23.3%	[19]
Tetrahydrofuran	Sulfolane	303.1	2.34	2.56	9.3%	M.G.	N.A.	[13]
Tetrahydrofuran	Sulfolane	317.9	2.30	2.38	3.6%	M.G.	N.A.	[13]
Tetrahydrofuran	Sulfolane	333.6	2.24	2.21	-1.3%	M.G.	N.A.	[13]
Tetrahydrofuran	Tetraethylene Glycol DME	303.2	0.80	0.82	2.0%	0.72	-10.4%	[7]
Tetrahydrofuran	Tetraethylene Glycol DME	323.2	0.78	0.81	4.2%	0.69	-11.2%	[7]
Tetrahydrofuran	Tetraethylene Glycol DME	343.2	0.75	0.80	6.1%	0.67	-11.1%	[7]
Toluene	1,1-Dichloroethane	298.2	0.97	1.12	15.5%	0.92	-5.2%	[16]
Toluene	1,4-Dioxane	298.2	1.18	1.12	-5.1%	1.47	24.6%	[16]
Toluene	1,5-Dimethyl-2-Pyrrolidinone	298.2	1.11	1.22	9.9%	M.G.	N.A.	[29]
Toluene	1,5-Dimethyl-2-Pyrrolidinone	308.2	1.17	1.21	3.4%	M.G.	N.A.	[29]
Toluene	1,5-Dimethyl-2-Pyrrolidinone	318.2	1.24	1.21	-2.4%	M.G.	N.A.	[29]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Toluene	1-Butanol	298.2	3.42	3.06	-10.5%	3.35	-2.0%	[16]
Toluene	1-Butanol	308.2	3.19	3.00	-6.0%	3.25	1.9%	[30]
Toluene	1-Butanol	318.2	3.30	2.93	-11.2%	3.15	-4.5%	[30]
Toluene	1-Butanol	323.2	3.33	2.90	-12.9%	3.10	-6.9%	[24]
Toluene	1-Butanol	328.2	3.21	2.86	-10.9%	3.05	-5.0%	[30]
Toluene	1-Butanol	349.5	2.80	2.70	-3.6%	2.84	1.4%	[17]
Toluene	1-Butanol	359.9	2.61	2.62	0.4%	2.74	5.0%	[17]
Toluene	1-Butanol	363.2	2.77	2.59	-6.5%	2.71	-2.2%	[24]
Toluene	1-Butanol	373.2	2.66	2.52	-5.3%	2.62	-1.5%	[24]
Toluene	1-Butanol	381.0	2.40	2.46	2.5%	2.56	6.7%	[17]
Toluene	1-Butanol	383.2	2.43	2.44	0.4%	2.54	4.5%	[24]
Toluene	1-Butanol	389.9	2.27	2.40	5.7%	2.50	10.1%	[17]
Toluene	1-Butanol	390.2	2.34	2.40	2.6%	2.49	6.4%	[24]
Toluene	1-Ethylpyrrolidin-2-One	298.2	1.12	1.22	8.9%	0.89	-20.5%	[29]
Toluene	1-Ethylpyrrolidin-2-One	308.2	1.23	1.22	-0.8%	0.90	-26.8%	[29]
Toluene	1-Ethylpyrrolidin-2-One	318.2	1.32	1.22	-7.6%	0.92	-30.3%	[29]
Toluene	1-Hexanol	293.2	2.53	2.58	2.0%	2.46	-2.8%	[28]
Toluene	1-Hexanol	313.2	2.39	2.46	2.9%	2.30	-3.8%	[28]
Toluene	1-Hexanol	323.2	2.35	2.40	2.1%	2.22	-5.5%	[24]
Toluene	1-Hexanol	333.2	2.26	2.34	3.5%	2.14	-5.3%	[28]
Toluene	1-Octanol	293.4	2.02	1.98	-2.0%	1.99	-1.5%	[31]
Toluene	1-Octanol	298.2	2.04	1.95	-4.4%	1.95	-4.4%	[3]
Toluene	1-Octanol	298.2	2.11	1.95	-7.6%	1.95	-7.6%	[69]
Toluene	1-Octanol	298.2	2.00	1.95	-2.5%	1.95	-2.5%	[16]
Toluene	1-Octanol	298.2	2.18	1.95	-10.6%	1.95	-10.6%	[32]
Toluene	1-Octanol	303.5	2.02	1.92	-5.0%	1.91	-5.4%	[31]
Toluene	1-Octanol	313.6	1.90	1.87	-1.6%	1.84	-3.2%	[31]
Toluene	1-Octanol	323.4	1.83	1.82	-0.5%	1.78	-2.7%	[31]
Toluene	1-Pentanol	303.5	3.06	2.58	-15.7%	2.75	-10.1%	[33]
Toluene	1-Pentanol	308.2	3.02	2.55	-15.6%	2.71	-10.3%	[30]
Toluene	1-Pentanol	313.2	2.91	2.52	-13.4%	2.66	-8.6%	[33]
Toluene	1-Pentanol	318.2	3.05	2.49	-18.4%	2.62	-14.1%	[30]
Toluene	1-Pentanol	323.2	2.80	2.46	-12.1%	2.57	-8.2%	[24]
Toluene	1-Pentanol	323.5	2.86	2.46	-14.0%	2.57	-10.1%	[33]
Toluene	1-Pentanol	328.2	3.07	2.43	-20.8%	2.53	-17.6%	[30]
Toluene	1-Phenyl-1-Butanone	298.1	0.80	1.09	36.3%	1.03	28.8%	[34]
Toluene	1-Propanol	298.2	4.25	3.88	-8.7%	4.29	0.9%	[16]
Toluene	1-Propanol	343.2	4.00	3.42	-14.5%	3.75	-6.3%	[24]
Toluene	1-Propanol	353.2	3.73	3.31	-11.3%	3.62	-2.9%	[24]
Toluene	1-Propanol	363.2	3.54	3.19	-9.9%	3.50	-1.1%	[24]
Toluene	1-Propanol	370.2	3.36	3.12	-7.1%	3.42	1.8%	[24]
Toluene	2,2,4-Trimethylpentane	298.2	1.57	1.84	17.2%	1.49	-5.1%	[16]
Toluene	2,2,4-Trimethylpentane	313.2	1.52	1.75	15.2%	1.43	-5.9%	99
Toluene	2,6-Dimethylpyridine	298.2	0.90	1.10	22.2%	1.00	11.1%	[16]
Toluene	2-Methyl-1-Propanol	313.2	4.07	3.14	-22.9%	3.20	-21.5%	22
Toluene	2-Methyl-2-Propanol	298.2	4.04	2.61	-35.4%	3.57	-11.6%	[16]
Toluene	2-Methyl-2-Propanol	313.2	3.46	2.52	-27.1%	3.41	-1.3%	19
Toluene	2-Pyrrolidone	303.2	4.00	4.34	8.4%	M.G.	N.A.	[35]
Toluene	2-Pyrrolidone	313.2	4.04	4.05	0.3%	M.G.	N.A.	[35]
Toluene	2-Pyrrolidone	323.2	4.06	3.79	-6.7%	M.G.	N.A.	[35]
Toluene	2-Pyrrolidone	333.2	4.09	3.57	-12.6%	M.G.	N.A.	[35]
Toluene	Acetic Acid	298.2	4.63	4.39	-5.2%	4.57	-1.3%	[16]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Toluene	Acetone	298.2	1.89	1.90	0.5%	1.72	-9.0%	[16]
Toluene	Acetone	298.3	2.09	1.90	-9.1%	1.72	-17.7%	[17]
Toluene	Acetone	308.2	2.03	1.86	-8.4%	1.70	-16.3%	[17]
Toluene	Acetone	318.4	1.89	1.81	-4.2%	1.68	-11.1%	[17]
Toluene	Acetone	328.5	1.78	1.77	-0.6%	1.66	-6.7%	[17]
Toluene	Acetonitrile	293.2	4.45	4.55	2.3%	3.97	-10.7%	373
Toluene	Acetonitrile	298.2	4.03	4.35	7.9%	3.89	-3.5%	[63]
Toluene	Acetonitrile	298.2	4.30	4.35	1.2%	3.89	-9.5%	[64]
Toluene	Acetonitrile	298.2	4.23	4.35	2.8%	3.89	-8.0%	[16]
Toluene	Acetonitrile	343.2	3.59	3.09	-13.9%	3.35	-6.7%	373
Toluene	Acetonitrile	393.2	3.08	2.36	-23.5%	2.95	-4.3%	373
Toluene	Acetophenone	298.2	1.26	1.46	15.9%	1.48	17.5%	[16]
Toluene	Alpha-Pinene	353.2	1.35	1.21	-10.4%	1.09	-19.3%	[22]
Toluene	Alpha-Pinene	373.2	1.38	1.18	-14.5%	1.06	-23.2%	[22]
Toluene	Aniline	298.2	2.84	2.70	-4.9%	2.47	-13.0%	[16]
Toluene	Anisole	298.2	1.02	1.15	12.7%	1.05	2.9%	[16]
Toluene	Benzene	298.2	0.92	1.00	8.7%	1.01	9.8%	[16]
Toluene	Benzonitrile	298.2	1.31	1.56	19.1%	M.G.	N.A.	[16]
Toluene	Benzonitrile	323.2	1.33	1.48	11.0%	M.G.	N.A.	288
Toluene	Benzonitrile	353.2	1.32	1.42	7.3%	M.G.	N.A.	288
Toluene	Benzyl Alcohol	298.2	2.73	2.43	-11.0%	2.44	-10.6%	[16]
Toluene	Bromobenzene	298.2	1.01	1.02	1.0%	0.95	-5.9%	[16]
Toluene	Bromoethane	298.2	1.07	1.03	-3.7%	1.02	-4.7%	[16]
Toluene	Butyl Ether	298.2	1.01	1.02	1.0%	1.07	5.9%	[16]
Toluene	Butyronitrile	298.2	1.50	1.62	8.0%	2.97	98.0%	[16]
Toluene	Carbon Disulfide	298.2	1.47	1.49	1.4%	1.14	-22.4%	[16]
Toluene	Carbon Disulfide	298.3	1.96	1.49	-24.0%	1.14	-41.8%	[17]
Toluene	Carbon Disulfide	308.4	1.86	1.46	-21.5%	1.12	-39.8%	[17]
Toluene	Carbon Disulfide	318.7	1.73	1.43	-17.3%	1.12	-35.3%	[17]
Toluene	Carbon Tetrachloride	298.2	1.02	1.02	0.0%	1.02	0.0%	[16]
Toluene	Carbon Tetrachloride	313.2	1.05	1.02	-3.3%	1.02	-3.3%	90
Toluene	Chlorobenzene	298.2	0.96	1.02	6.3%	0.97	1.0%	[16]
Toluene	Chloroform	298.2	0.68	0.70	2.9%	0.76	11.8%	[16]
Toluene	Chloroform	318.2	0.82	0.74	-9.6%	0.81	-1.1%	233
Toluene	Cyclohexane	298.2	1.57	1.51	-3.8%	1.54	-1.9%	[16]
Toluene	Cyclohexanone	298.2	1.01	1.11	9.9%	1.10	8.9%	[16]
Toluene	Dichloromethane	298.2	0.86	0.95	10.5%	1.03	19.8%	203
Toluene	Dichloromethane	298.2	0.96	0.95	-1.0%	1.03	7.3%	[16]
Toluene	Dichloromethane	347.9	0.91	0.95	4.5%	1.07	17.7%	203
Toluene	Diethyl Ether	298.2	1.20	1.23	2.5%	1.31	9.2%	[16]
Toluene	Diethyl Phthalate	303.2	1.09	1.14	4.6%	M.G.	N.A.	[39]
Toluene	Diethyl Phthalate	313.2	1.08	1.12	3.7%	M.G.	N.A.	[39]
Toluene	Diethyl Phthalate	323.2	1.09	1.11	1.8%	M.G.	N.A.	[39]
Toluene	Diethyl Phthalate	333.2	1.09	1.09	0.0%	M.G.	N.A.	[39]
Toluene	Diiodomethane	298.2	3.86	3.53	-8.5%	M.G.	N.A.	[16]
Toluene	Diisopropyl Ether	298.2	1.24	1.09	-12.1%	1.23	-0.8%	[16]
Toluene	Dimethyl Carbonate	318.2	2.66	1.45	-45.4%	M.G.	N.A.	306
Toluene	Dimethyl Sulfoxide	298.2	4.41	3.50	-20.6%	4.44	0.7%	[16]
Toluene	Epsilon-Caprolactone	303.2	1.83	1.92	4.9%	M.G.	N.A.	[41]
Toluene	Epsilon-Caprolactone	318.2	1.82	1.83	0.5%	M.G.	N.A.	[41]
Toluene	Epsilon-Caprolactone	333.2	1.82	1.76	-3.3%	M.G.	N.A.	[41]
Toluene	Ethanol	296.4	7.80	5.68	-27.2%	6.28	-19.5%	[48]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Toluene	Ethanol	298.2	5.77	5.66	-1.9%	6.25	8.3%	[16]
Toluene	Ethanol	303.2	5.97	5.59	-6.4%	6.17	3.4%	211
Toluene	Ethanol	313.2	5.74	5.43	-5.4%	6.02	4.8%	211
Toluene	Ethanol	318.5	5.60	5.34	-4.6%	5.93	5.9%	[58]
Toluene	Ethanol	318.5	5.60	5.34	-4.6%	5.93	5.9%	[12]
Toluene	Ethanol	318.6	7.00	5.33	-23.9%	5.92	-15.4%	[48]
Toluene	Ethanol	318.6	6.90	5.33	-22.8%	5.92	-14.2%	[48]
Toluene	Ethanol	323.2	5.53	5.25	-5.1%	5.84	5.5%	211
Toluene	Ethanol	323.2	5.84	5.25	-10.1%	5.84	0.0%	[24]
Toluene	Ethanol	330.0	5.34	5.11	-4.3%	5.72	7.1%	[12]
Toluene	Ethanol	333.2	5.37	5.05	-5.9%	5.66	5.5%	211
Toluene	Ethanol	333.2	5.64	5.05	-10.5%	5.66	0.4%	[24]
Toluene	Ethanol	337.2	6.00	4.96	-17.3%	5.59	-6.8%	[48]
Toluene	Ethanol	343.2	5.39	4.84	-10.2%	5.47	1.5%	[24]
Toluene	Ethanol	349.4	5.14	4.70	-8.6%	5.35	4.1%	[12]
Toluene	Ethanol	351.2	5.19	4.67	-10.0%	5.31	2.3%	[24]
Toluene	Ethanol	351.8	5.60	4.65	-17.0%	5.30	-5.4%	[48]
Toluene	Ethyl Acetate	298.2	1.33	1.28	-3.8%	1.43	7.5%	[16]
Toluene	Ethyl Acetate	313.0	1.27	1.27	0.0%	1.40	10.2%	[12]
Toluene	Ethyl Acetate	328.4	1.23	1.26	2.4%	1.37	11.4%	[17]
Toluene	Ethyl Acetate	333.5	1.18	1.25	5.9%	1.36	15.3%	[12]
Toluene	Ethyl Acetate	338.4	1.20	1.25	4.2%	1.36	13.3%	[17]
Toluene	Ethyl Acetate	348.3	1.14	1.24	8.8%	1.34	17.5%	[12]
Toluene	Ethyl Acetate	349.1	1.16	1.24	6.9%	1.34	15.5%	[17]
Toluene	Ethyl Benzoate	313.2	1.04	1.04	0.0%	M.G.	N.A.	[41]
Toluene	Ethyl Benzoate	323.2	1.04	1.04	0.0%	M.G.	N.A.	[41]
Toluene	Ethyl Benzoate	333.2	1.03	1.03	0.0%	M.G.	N.A.	[41]
Toluene	Ethyl Benzoate	343.2	1.03	1.03	0.0%	M.G.	N.A.	[41]
Toluene	Glutaronitrile	303.2	5.21	5.67	8.8%	M.G.	N.A.	[39]
Toluene	Glutaronitrile	313.2	5.05	5.17	2.4%	M.G.	N.A.	[39]
Toluene	Glutaronitrile	323.2	4.95	4.75	-4.0%	M.G.	N.A.	[39]
Toluene	Glutaronitrile	333.2	4.81	4.39	-8.7%	M.G.	N.A.	[39]
Toluene	Isopropanol	298.2	5.08	4.04	-20.5%	4.15	-18.3%	[63]
Toluene	Isopropanol	298.2	5.30	4.04	-23.8%	4.15	-21.7%	[64]
Toluene	Isopropanol	298.2	5.18	4.04	-22.0%	4.15	-19.9%	[16]
Toluene	Isopropanol	313.2	4.97	3.88	-21.9%	3.98	-19.9%	[17]
Toluene	Isopropanol	321.0	4.66	3.79	-18.7%	3.89	-16.5%	[17]
Toluene	Isopropanol	331.7	4.34	3.66	-15.7%	3.76	-13.4%	[17]
Toluene	Isopropanol	343.1	4.08	3.52	-13.7%	3.62	-11.3%	[17]
Toluene	Isopropanol	354.8	3.63	3.38	-6.9%	3.48	-4.1%	[17]
Toluene	M-Cresol	298.2	2.35	1.58	-32.8%	2.19	-6.8%	[16]
Toluene	Methanol	298.2	9.67	9.38	-3.0%	9.81	1.4%	[63]
Toluene	Methanol	298.2	10.10	9.38	-7.1%	9.81	-2.9%	[64]
Toluene	Methanol	298.2	10.04	9.38	-6.6%	9.81	-2.3%	[16]
Toluene	Methanol	303.2	9.97	9.22	-7.5%	9.68	-2.9%	[69]
Toluene	Methanol	307.2	9.84	9.08	-7.7%	9.58	-2.6%	[82]
Toluene	Methanol	308.2	10.10	9.04	-10.5%	9.55	-5.4%	[24]
Toluene	Methanol	308.7	9.70	9.02	-7.0%	9.54	-1.6%	[17]
Toluene	Methanol	318.2	9.77	8.63	-11.7%	9.29	-4.9%	[24]
Toluene	Methanol	318.5	9.42	8.62	-8.5%	9.29	-1.4%	[17]
Toluene	Methanol	328.2	9.43	8.17	-13.4%	9.04	-4.1%	[24]
Toluene	Methanol	328.5	9.15	8.16	-10.8%	9.03	-1.3%	[17]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Toluene	Methanol	337.0	8.90	7.76	-12.8%	8.81	-1.0%	[17]
Toluene	Methanol	337.2	9.21	7.75	-15.9%	8.80	-4.5%	[24]
Toluene	Methyl Ethyl Ketone	298.2	1.33	1.31	-1.5%	1.42	6.8%	[16]
Toluene	Methyl Ethyl Ketone	323.2	1.26	1.28	1.6%	1.40	11.1%	591
Toluene	Methylcyclohexane	343.2	1.33	1.36	2.3%	1.31	-1.5%	[83]
Toluene	Methylcyclohexane	353.2	1.30	1.34	3.1%	1.28	-1.5%	[83]
Toluene	N,N-Dibutylformamide	302.8	0.92	0.88	-4.6%	0.85	-7.8%	[13]
Toluene	N,N-Dibutylformamide	318.3	0.95	0.88	-7.6%	0.85	-10.7%	[13]
Toluene	N,N-Dibutylformamide	332.4	0.98	0.89	-8.8%	0.85	-12.9%	[13]
Toluene	N,N-Diethylacetamide	303.2	1.20	1.15	-4.2%	0.99	-17.5%	[39]
Toluene	N,N-Diethylacetamide	313.2	1.20	1.15	-4.2%	0.99	-17.5%	[39]
Toluene	N,N-Diethylacetamide	323.2	1.20	1.14	-5.0%	1.00	-16.7%	[39]
Toluene	N,N-Diethylacetamide	333.2	1.20	1.14	-5.0%	1.00	-16.7%	[39]
Toluene	N,N-Dimethylacetamide	303.6	1.49	1.51	1.7%	1.41	-5.1%	[13]
Toluene	N,N-Dimethylacetamide	317.6	1.47	1.48	1.0%	1.40	-4.5%	[13]
Toluene	N,N-Dimethylacetamide	333.2	1.45	1.45	0.2%	1.39	-3.9%	[13]
Toluene	N,N-Dimethylformamide	298.2	1.91	2.36	23.6%	2.18	14.1%	[16]
Toluene	N-Decane	298.2	1.26	1.37	8.7%	1.34	6.3%	[16]
Toluene	N-Ethylacetamide	303.2	3.12	2.70	-13.5%	M.G.	N.A.	[39]
Toluene	N-Ethylacetamide	313.2	3.12	2.64	-15.4%	M.G.	N.A.	[39]
Toluene	N-Ethylacetamide	323.2	3.12	2.59	-17.0%	M.G.	N.A.	[39]
Toluene	N-Ethylacetamide	333.2	3.13	2.52	-19.5%	M.G.	N.A.	[39]
Toluene	N-Formylmorpholine	313.3	2.78	3.53	27.0%	M.G.	N.A.	[43]
Toluene	N-Formylmorpholine	332.7	2.65	3.16	19.2%	M.G.	N.A.	[43]
Toluene	N-Formylmorpholine	352.5	2.58	2.85	10.5%	M.G.	N.A.	[43]
Toluene	N-Formylmorpholine	373.4	2.46	2.60	5.7%	M.G.	N.A.	[43]
Toluene	N-Heptane	298.2	1.51	1.58	4.6%	1.59	5.3%	[16]
Toluene	N-Hexadecane	298.2	1.00	1.09	9.2%	1.05	5.2%	[6]
Toluene	N-Hexadecane	298.2	0.96	1.09	13.5%	1.05	9.4%	[16]
Toluene	N-Hexadecane	333.2	0.90	1.01	12.2%	0.96	6.7%	[71]
Toluene	N-Hexadecane	393.2	0.81	0.92	13.6%	0.86	6.2%	[71]
Toluene	N-Hexadecane	453.2	0.76	0.86	13.2%	0.79	3.9%	[71]
Toluene	N-Hexane	298.2	1.64	1.68	2.4%	1.73	5.5%	[16]
Toluene	N-Hexane	304.8	1.59	1.65	3.8%	1.69	6.3%	[12]
Toluene	N-Hexane	322.8	1.46	1.57	7.5%	1.62	11.0%	[12]
Toluene	Nitrobenzene	298.2	1.40	1.61	15.0%	1.54	10.0%	[16]
Toluene	Nitromethane	298.2	5.10	5.14	0.8%	4.99	-2.2%	[16]
Toluene	Nitromethane	343.2	4.30	3.52	-18.1%	3.77	-12.3%	[83]
Toluene	Nitromethane	353.2	4.13	3.29	-20.3%	3.57	-13.6%	[83]
Toluene	N-Methyl-2-Pyrrolidone	323.4	1.66	1.42	-14.5%	1.19	-28.3%	[43]
Toluene	N-Methyl-2-Pyrrolidone	333.2	1.67	1.41	-15.6%	1.21	-27.5%	[43]
Toluene	N-Methyl-2-Pyrrolidone	343.4	1.66	1.40	-15.7%	1.22	-26.5%	[43]
Toluene	N-Methyl-2-Pyrrolidone	363.3	1.08	1.37	27.1%	1.25	16.0%	238
Toluene	N-Methyl-2-Pyrrolidone	383.4	1.07	1.35	26.2%	1.27	18.7%	238
Toluene	N-Methylacetamide	303.2	3.81	3.62	-4.9%	3.81	0.1%	[13]
Toluene	N-Methylacetamide	318.4	3.71	3.48	-6.1%	3.73	0.6%	[13]
Toluene	N-Methylacetamide	333.2	3.62	3.32	-8.2%	3.67	1.4%	[13]
Toluene	N-Methylformamide	303.2	7.26	6.74	-7.2%	M.P.	N.A.	[35]
Toluene	N-Methylformamide	313.2	7.14	6.38	-10.6%	M.P.	N.A.	[35]
Toluene	N-Methylformamide	323.2	7.00	6.02	-14.0%	M.P.	N.A.	[35]
Toluene	N-Methylformamide	333.2	6.88	5.67	-17.5%	M.P.	N.A.	[35]
Toluene	N-Octane	333.2	1.31	1.38	5.6%	1.36	4.0%	332

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Toluene	N-Pentane	298.2	1.94	1.85	-4.6%	1.91	-1.5%	[16]
Toluene	Phenol	323.2	2.62	2.57	-1.9%	2.45	-6.5%	[10]
Toluene	Phenol	328.2	3.45	2.54	-26.4%	2.41	-30.1%	[14]
Toluene	Phenol	343.2	3.00	2.46	-18.0%	2.30	-23.3%	[14]
Toluene	Phenol	358.2	2.89	2.37	-18.0%	2.19	-24.2%	[14]
Toluene	Phenol	373.2	2.84	2.28	-19.7%	2.08	-26.8%	[14]
Toluene	P-Xylene	298.2	0.97	1.02	5.2%	1.00	3.1%	[16]
Toluene	Pyridine	293.2	1.35	1.57	16.6%	1.53	13.7%	238
Toluene	Pyridine	298.2	1.30	1.55	19.2%	1.52	16.9%	238
Toluene	Pyridine	298.2	1.33	1.55	17.0%	1.52	14.7%	238
Toluene	Pyridine	298.2	1.42	1.55	9.2%	1.52	7.0%	[16]
Toluene	Pyridine	303.2	1.31	1.53	16.4%	1.52	15.6%	238
Toluene	Pyridine	303.2	1.36	1.53	12.2%	1.52	11.4%	238
Toluene	Pyridine	308.2	1.33	1.51	13.4%	1.51	13.4%	238
Toluene	Pyridine	313.2	1.32	1.50	13.3%	1.51	14.1%	238
Toluene	Pyridine	313.2	1.34	1.50	11.9%	1.51	12.6%	238
Toluene	Pyridine	323.2	1.32	1.46	10.3%	1.49	12.6%	238
Toluene	Pyridine	333.2	1.32	1.43	8.3%	1.48	12.0%	238
Toluene	Pyridine	373.2	1.31	1.33	1.9%	1.42	8.8%	238
Toluene	Sulfolane	303.8	3.61	3.97	9.9%	M.G.	N.A.	[13]
Toluene	Sulfolane	317.9	3.49	3.57	2.2%	M.G.	N.A.	[13]
Toluene	Sulfolane	333.6	3.36	3.21	-4.4%	M.G.	N.A.	[13]
Toluene	Tetraethylene Glycol DME	313.2	0.85	0.91	7.3%	0.80	-5.7%	[7]
Toluene	Tetraethylene Glycol DME	323.2	0.86	0.91	6.1%	0.80	-6.8%	[7]
Toluene	Tetraethylene Glycol DME	343.2	0.89	0.91	2.1%	0.79	-11.3%	[7]
Toluene	Tetrahydrofuran	298.2	0.84	0.87	3.6%	0.75	-10.7%	[63]
Toluene	Tetrahydrofuran	298.2	0.84	0.87	3.6%	0.75	-10.7%	[64]
Toluene	Tetrahydrofuran	298.2	0.82	0.87	6.1%	0.75	-8.5%	[16]
Toluene	Tributyl Phosphate	298.2	0.70	0.62	-11.4%	M.G.	N.A.	[20]
Toluene	Tributyl Phosphate	298.6	0.70	0.62	-11.4%	M.G.	N.A.	[27]
Toluene	Tributyl Phosphate	302.9	0.71	0.62	-12.7%	M.G.	N.A.	[27]
Toluene	Tributyl Phosphate	308.6	0.73	0.62	-15.1%	M.G.	N.A.	[27]
Toluene	Tributyl Phosphate	313.1	0.74	0.63	-14.9%	M.G.	N.A.	[27]
Toluene	Tributyl Phosphate	318.2	0.70	0.63	-10.0%	M.G.	N.A.	[20]
Toluene	Tributyl Phosphate	323.7	0.79	0.63	-20.3%	M.G.	N.A.	[27]
Toluene	Tributyl Phosphate	333.2	0.69	0.64	-7.2%	M.G.	N.A.	[20]
Toluene	Tributyl Phosphate	333.2	0.73	0.64	-12.3%	M.G.	N.A.	[73]
Toluene	Triethylamine	298.2	1.21	1.22	0.8%	1.22	0.8%	[16]
Trichloroethylene	1,1,1-Trichloroethane	328.2	1.00	0.99	-1.0%	1.39	39.0%	[9]
Trichloroethylene	1,2-Dichloroethane	328.2	1.45	1.30	-10.3%	1.04	-28.3%	[9]
Trichloroethylene	1-Octanol	298.2	1.60	1.59	-0.6%	2.01	25.6%	[4]
Trichloroethylene	Carbon Tetrachloride	328.2	0.99	1.04	5.1%	1.08	9.1%	[9]
Trichloroethylene	Chloroform	328.2	1.07	1.13	5.6%	1.26	17.8%	[9]
Trichloroethylene	Dichloromethane	308.2	1.46	1.31	-10.3%	1.54	5.5%	[9]
Trichloroethylene	N,N-Dibutylformamide	302.8	0.57	0.49	-13.9%	0.52	-8.6%	[13]
Trichloroethylene	N,N-Dibutylformamide	318.3	0.59	0.53	-9.9%	0.54	-8.2%	[13]
Trichloroethylene	N,N-Dibutylformamide	332.4	0.62	0.55	-10.7%	0.54	-12.3%	[13]
Trichloroethylene	N,N-Dimethylacetamide	303.6	0.85	0.93	9.7%	M.P.	N.A.	[13]
Trichloroethylene	N,N-Dimethylacetamide	317.6	0.92	0.97	5.1%	M.P.	N.A.	[13]
Trichloroethylene	N,N-Dimethylacetamide	333.0	1.01	1.00	-1.3%	M.P.	N.A.	[13]
Trichloroethylene	N-Methylacetamide	303.4	2.18	2.58	18.3%	M.P.	N.A.	[13]
Trichloroethylene	N-Methylacetamide	318.4	2.30	2.50	8.6%	M.P.	N.A.	[13]

Solute	Solvent	T (K)	EXP	MOS	Error	UNI	Error	Ref.
Trichloroethylene	N-Methylacetamide	333.2	2.43	2.41	-0.9%	M.P.	N.A.	[13]
Trichloroethylene	Sulfolane	303.1	3.26	3.40	4.2%	M.G.	N.A.	[13]
Trichloroethylene	Sulfolane	317.9	3.09	3.10	0.3%	M.G.	N.A.	[13]
Trichloroethylene	Sulfolane	332.6	2.94	2.86	-2.8%	M.G.	N.A.	[13]
Trichloroethylene	Tetraethylene Glycol DME	303.2	0.53	0.56	5.7%	0.30	-43.4%	[7]
Trichloroethylene	Tetraethylene Glycol DME	323.2	0.57	0.59	3.0%	0.42	-26.7%	[7]
Trichloroethylene	Tetraethylene Glycol DME	343.2	0.65	0.62	-5.1%	0.54	-17.3%	[7]
Triethylamine	1,2-Dichloroethane	293.2	2.14	1.65	-22.9%	1.15	-46.3%	[10]
Triethylamine	1,2-Dichloroethane	310.9	2.05	1.62	-21.0%	1.11	-45.9%	[12]
Triethylamine	1,2-Dichloroethane	329.0	1.96	1.58	-19.4%	1.06	-45.9%	[12]
Triethylamine	1,2-Dichloroethane	354.2	1.82	1.53	-15.9%	0.99	-45.6%	[12]
Triethylamine	1-Chlorobutane	311.4	1.14	1.27	11.4%	M.P.	N.A.	[12]
Triethylamine	1-Chlorobutane	349.0	1.11	1.22	9.9%	M.P.	N.A.	[12]
Triethylamine	Acetone	304.7	3.95	3.88	-1.8%	3.97	0.5%	[12]
Triethylamine	Acetone	315.7	3.73	3.57	-4.3%	3.74	0.3%	[12]
Triethylamine	Acetone	326.7	3.50	3.31	-5.4%	3.53	0.9%	[12]
Triethylamine	Acetonitrile	293.2	11.10	10.98	-1.1%	M.P.	N.A.	[10]
Triethylamine	Benzene	336.7	1.24	1.35	8.9%	1.35	8.9%	[12]
Triethylamine	Benzene	352.4	1.21	1.32	9.1%	1.31	8.3%	[12]
Triethylamine	Carbon Tetrachloride	321.7	0.75	0.81	8.0%	0.79	5.3%	[12]
Triethylamine	Carbon Tetrachloride	335.2	0.79	0.84	6.3%	0.82	3.8%	[12]
Triethylamine	Carbon Tetrachloride	347.1	0.81	0.85	4.9%	0.85	4.9%	[12]
Triethylamine	Chloroform	283.1	0.13	0.14	6.6%	0.15	14.2%	113
Triethylamine	Chloroform	323.0	0.27	0.25	-7.4%	0.32	18.5%	[12]
Triethylamine	Cyclohexanone	293.2	2.59	3.13	20.8%	M.P.	N.A.	[10]
Triethylamine	Dichloromethane	283.2	1.21	0.65	-46.5%	0.93	-23.4%	112
Triethylamine	Ethyl Acetate	293.2	2.43	2.32	-4.5%	2.38	-2.1%	[10]
Triethylamine	Ethyl Acetate	306.2	2.04	2.19	7.4%	2.19	7.4%	[12]
Triethylamine	Ethyl Acetate	321.2	1.94	2.07	6.7%	2.00	3.1%	[12]
Triethylamine	Ethyl Acetate	342.7	1.84	1.92	4.3%	1.78	-3.3%	[12]
Triethylamine	Methyl Ethyl Ketone	293.2	2.79	2.88	3.2%	2.96	6.1%	[10]
Triethylamine	Methyl Ethyl Ketone	316.0	2.48	2.54	2.4%	2.72	9.7%	[12]
Triethylamine	Methyl Ethyl Ketone	341.3	2.21	2.27	2.7%	2.49	12.7%	[12]
Triethylamine	Methyl Ethyl Ketone	352.0	2.12	2.18	2.8%	2.41	13.7%	[12]
Triethylamine	N-Hexane	298.0	1.10	1.07	-2.7%	1.07	-2.7%	[12]
Triethylamine	N-Hexane	322.9	1.10	1.06	-3.6%	1.06	-3.6%	[12]
Triethylamine	N-Hexane	330.1	1.03	1.06	2.9%	1.06	2.9%	[12]
Triethylamine	N-Hexane	340.7	1.06	1.05	-0.9%	1.05	-0.9%	[12]
Triethylamine	Nitrobenzene	293.2	4.05	4.34	7.2%	M.P.	N.A.	[10]
Triethylamine	Nitromethane	293.2	12.80	12.49	-2.4%	M.P.	N.A.	[10]
Triethylamine	Propionitrile	293.2	4.40	6.64	50.9%	M.P.	N.A.	[10]
Triethylamine	P-Xylene	293.2	1.08	1.19	10.2%	1.10	1.9%	[10]
Triethylamine	Toluene	293.2	1.21	1.30	7.4%	1.17	-3.3%	[10]

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212	Int. Data Ser., Selec. Data Mixtures, Ser. A		4	1977
213	Int. Data Ser., Selec. Data Mixtures, Ser. A		56	1978
214	Int. Data Ser., Selec. Data Mixtures, Ser. A		62	1978
215	Int. Data Ser., Selec. Data Mixtures, Ser. A		65	1978
216	Int. Data Ser., Selec. Data Mixtures, Ser. A		68	1978
217	Int. Data Ser., Selec. Data Mixtures, Ser. A		102	1978
218	Int. Data Ser., Selec. Data Mixtures, Ser. A		42	1979
219	Int. Data Ser., Selec. Data Mixtures, Ser. A		87	1983
220	Int. Data Ser., Selec. Data Mixtures, Ser. A		93	1983
221	Int. Data Ser., Selec. Data Mixtures, Ser. A		17	1984
222	Int. Data Ser., Selec. Data Mixtures, Ser. A		18	1984
223	Int. Data Ser., Selec. Data Mixtures, Ser. A		19	1984
224	Int. Data Ser., Selec. Data Mixtures, Ser. A		20	1984
225	Int. Data Ser., Selec. Data Mixtures, Ser. A		93	1987
226	Int. Data Ser., Selec. Data Mixtures, Ser. A		96	1987
227	Int. Data Ser., Selec. Data Mixtures, Ser. A		218	1997
228	Int. Data Ser., Selec. Data Mixtures, Ser. A		253	1998
229	Int. Data Ser., Selec. Data Mixtures, Ser. A		256	1998
230	Int. Data Ser., Selec. Data Mixtures, Ser. A		274	1998
231	Int. Data Ser., Selec. Data Mixtures, Ser. A		277	1998
232	Int. Data Ser., Selec. Data Mixtures, Ser. A		291	1998
233	Int. Data Ser., Selec. Data Mixtures, Ser. A		295	1998
234	Int. Data Ser., Selec. Data Mixtures, Ser. A		299	1998
235	Int. Data Ser., Selec. Data Mixtures, Ser. A		3	1999
236	Int. Data Ser., Selec. Data Mixtures, Ser. A		72	1999
237	Int. Data Ser., Selec. Data Mixtures, Ser. A		75	1999
238	Int. Data Ser., Selec. Data Mixtures, Ser. A		258	1993
239	Int. Data Ser., Selec. Data Mixtures, Ser. A		246	1993
240	Int. Data Ser., Selec. Data Mixtures, Ser. A		190	1993
241	Int. Data Ser., Selec. Data Mixtures, Ser. A		184	1993
242	Int. Data Ser., Selec. Data Mixtures, Ser. A		172	1993
243	Int. Data Ser., Selec. Data Mixtures, Ser. A		302	1998
244	Int. Data Ser., Selec. Data Mixtures, Ser. A		280	1998
245	Int. Data Ser., Selec. Data Mixtures, Ser. A		219	1998
246	Int. Data Ser., Selec. Data Mixtures, Ser. A		217	1998
247	Int. Data Ser., Selec. Data Mixtures, Ser. A		215	1998
248	Int. Data Ser., Selec. Data Mixtures, Ser. A		213	1998
249	Int. Data Ser., Selec. Data Mixtures, Ser. A		131	1998
250	Int. Data Ser., Selec. Data Mixtures, Ser. A		122	1998
251	Int. Data Ser., Selec. Data Mixtures, Ser. A		116	1998
252	Int. Data Ser., Selec. Data Mixtures, Ser. A		110	1998
253	Int. Data Ser., Selec. Data Mixtures, Ser. A		251	2001
254	Int. Data Ser., Selec. Data Mixtures, Ser. A		305	2000
255	Int. Data Ser., Selec. Data Mixtures, Ser. A		293	2000
256	Int. Data Ser., Selec. Data Mixtures, Ser. A		289	2000
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258	Int. Data Ser., Selec. Data Mixtures, Ser. A		248	2000
259	Int. Data Ser., Selec. Data Mixtures, Ser. A		241	2000
260	Int. Data Ser., Selec. Data Mixtures, Ser. A		242	1986
261	Int. Data Ser., Selec. Data Mixtures, Ser. A		212	2000
262	Int. Data Ser., Selec. Data Mixtures, Ser. A		254	2001
263	Int. Data Ser., Selec. Data Mixtures, Ser. A		243	1999
264	Int. Data Ser., Selec. Data Mixtures, Ser. A		234	1999
265	Int. Data Ser., Selec. Data Mixtures, Ser. A		237	1999
266	Int. Data Ser., Selec. Data Mixtures, Ser. A		204	2001
267	Int. Data Ser., Selec. Data Mixtures, Ser. A		92	1997
268	Int. Data Ser., Selec. Data Mixtures, Ser. A		95	1997
269	Int. Data Ser., Selec. Data Mixtures, Ser. A		89	1997
270	Int. Data Ser., Selec. Data Mixtures, Ser. A		251	2000
271	Int. Data Ser., Selec. Data Mixtures, Ser. A		118	1996
272	Int. Data Ser., Selec. Data Mixtures, Ser. A		114	1996
273	Int. Data Ser., Selec. Data Mixtures, Ser. A		110	1996
274	Int. Data Ser., Selec. Data Mixtures, Ser. A		108	1996
275	Int. Data Ser., Selec. Data Mixtures, Ser. A		120	1996
276	Int. Data Ser., Selec. Data Mixtures, Ser. A		4	1992
277	Int. Data Ser., Selec. Data Mixtures, Ser. A		242	1995
278	Int. Data Ser., Selec. Data Mixtures, Ser. A		307	1996
279	Int. Data Ser., Selec. Data Mixtures, Ser. A		76	2000
280	Int. Data Ser., Selec. Data Mixtures, Ser. A		74	2000
281	Int. Data Ser., Selec. Data Mixtures, Ser. A		65	2001
282	Int. Data Ser., Selec. Data Mixtures, Ser. A		238	2000
283	Int. Data Ser., Selec. Data Mixtures, Ser. A		233	1988
284	Int. Data Ser., Selec. Data Mixtures, Ser. A		203	1998
285	Int. Data Ser., Selec. Data Mixtures, Ser. A		313	1996
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288	J. Chem. Eng. Data	44	539	1999
290	Fluid Phase Equilibria	168	259	2000
291	Fluid Phase Equilibria	192	49	2001
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296	Int. Data Ser., Selec. Data Mixtures, Ser. A		133	1976
297	Int. Data Ser., Selec. Data Mixtures, Ser. A		130	1976
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299	Int. Data Ser., Selec. Data Mixtures, Ser. A		103	1976
300	Int. Data Ser., Selec. Data Mixtures, Ser. A		97	1976
301	Int. Data Ser., Selec. Data Mixtures, Ser. A		116	1975
302	Int. Data Ser., Selec. Data Mixtures, Ser. A		113	1975
303	Int. Data Ser., Selec. Data Mixtures, Ser. A		110	1975
304	Int. Data Ser., Selec. Data Mixtures, Ser. A		92	1975
305	Int. Data Ser., Selec. Data Mixtures, Ser. A		89	1975
306	Int. Data Ser., Selec. Data Mixtures, Ser. A		9	1974
307	Int. Data Ser., Selec. Data Mixtures, Ser. A		25	1977
308	Int. Data Ser., Selec. Data Mixtures, Ser. A		13	1977
309	Int. Data Ser., Selec. Data Mixtures, Ser. A		7	1977
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311	Int. Data Ser., Selec. Data Mixtures, Ser. A		14	1982
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316	Int. Data Ser., Selec. Data Mixtures, Ser. A		74	1979
317	Int. Data Ser., Selec. Data Mixtures, Ser. A		71	1979
318	Int. Data Ser., Selec. Data Mixtures, Ser. A		43	1979
319	Int. Data Ser., Selec. Data Mixtures, Ser. A		41	1979
320	Int. Data Ser., Selec. Data Mixtures, Ser. A		1	1979
321	Int. Data Ser., Selec. Data Mixtures, Ser. A		53	1978
322	DIPPR Data Ser.		34	1994
323	AIChE Symp. Ser.	83	49	1988
324	AIChE Symp. Ser.	85	51	1989
325	Fluid Phase Equilibria	179	217	2001
326	J. Chem. Eng. Data	41	1434	1996
327	J. Chem. Eng. Data	42	875	1997
328	J. Chem. Eng. Data	42	597	1997
329	J. Chem. Thermodynamics	33	47	2001
330	Fluid Phase Equilibria	150-151	775	1998
331	J. Chem. Thermodynamics	17	843	1985
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333	Int. Data Ser., Selec. Data Mixtures, Ser. A		11	1982
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338	Fluid Phase Equilibria	147	195	1998
339	J. Chem. Eng. Data	44	193	1999
340	Fluid Phase Equilibria	137	173	1997
341	J. Chem. Eng. Data	28	27	1983
342	J. Chem. Eng. Data	21	310	1976
343	Fluid Phase Equilibria	18	197	1984
344	J. Chem. Eng. Data	28	36	1983
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352	Fluid Phase Equilibria	154	223	1999
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408	J. Chem. Eng. Data	35	266	1990
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410	J. Chem. Eng. Data	28	100	1983
411	J. Chem. Eng. Data	28	108	1983
412	J. Chem. Eng. Data	28	93	1983
413	J. Chem. Thermodynamics	33	523	2001
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415	Fluid Phase Equilibria	7	55	1981
416	Fluid Phase Equilibria	8	285	1982
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420	J. Chem. Eng. Data	40	679	1995

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426	Fluid Phase Equilibria	207	53	2003
427	Fluid Phase Equilibria	207	97	2003
428	Fluid Phase Equilibria	206	87	2003
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432	J. Chem. Thermodynamics	11	1137	1979
433	Fluid Phase Equilibria	208	115	2003
434	Fluid Phase Equilibria	208	223	2003
435	Thermochimica Acta	362	153	2000
436	Fluid Phase Equilibria	209	265	2003
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438	Fluid Phase Equilibia	201	135	2002
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444	J. Chem.Eng. Data	32	447	1987
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447	J. Chem.Eng. Data	27	55	1982
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449	J. Chem. Eng. Data	32	444	1987
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451	Fluid Phase Equilibria	138	131	1997
452	Fluid Phase Equilibria	162	211	1999
453	Fluid Phase Equilibria	130	231	1997
454	Fluid Phase Equilibria	101	237	1994
455	J. Chem. Eng. Data	37	337	1992
456	J. Chem. Eng. Data	36	303	1992
457	J. Chem. Eng. Data	34	305	1989
458	J. Chem. Eng. Data	44	926	1999
459	Ind. Eng. Chem. Res.	29	295	1990
460	Fluid Phase Equilibria	138	159	1997
461	Fluid Phase Equilibria	198	299	2002
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463	J. Chem. Eng. Data	47	1171	2002
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468	J. Supercritical Fluids	17	97	2000
469	Fluid Phase Equilibria	175	53	2000
470	J. Chem. Eng. Data	37	264	1992
471	Fluid Phase Equilibria	152	67	1998
472	Fluid Phase Equilibria	23	243	1985

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474	J. Chem. Eng. Data	41	831	1996
475	J. Chem. Eng. Data	43	954	1998
476	J. Chem. Eng. Data	25	246	1980
477	J. Chem. Eng. Data	41	324	1996
478	Fluid Phase Equilibria	77	241	1991
479	Fluid Phase Equilibria	163	119	1999
480	J. Supercritical Fluids	18	87	2000
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482	J. Supercritical Fluids	15	117	1999
483	J. Chem. Eng. Data	46	1589	2001
484	J. Chem. Eng. Data	47	161	2002
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487	Fluid Phase Equilibria	171	165	2000
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494	Fluid Phase Equilibria	44	105	1988
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496	Fluid Phase Equilibria	167	113	2000
497	J. Chem. Eng. Data	48	97	2003
498	J. Supercritical Fluids	7	115	1994
499	J. Chem. Eng. Data	21	53	1976
500	J. Chem. Eng. Data	32	369	1987
501	Fluid Phase Equilibria	34	83	1987
502	Fluid Phase Equilibria	74	235	1992
503	J. Chem. Eng. Data	36	23	1991
505	Fluid Phase Equilibria	97	167	1994
506	J. Chem. Eng. Data	29	269	1984
507	Fluid Phase Equilibria	32	295	1987
508	J. Chem. Thermodynamics	24	387	1992
509	J. Chem. Eng. Data	34	419	1989
510	J. Chem. Thermodyamics	21	915	1989
511	J. Chem. Eng. Data	34	319	1989
512	J. Chem. Eng. Data	18	416	1973
513	Fluid Phase Equilibria	33	109	1987
514	J. Chem .Eng. Data	26	53	1981
515	J. Chem. Eng. Data	35	26	1990
516	J. Chem. Eng. Data	31	168	1986
517	Can. J. Chem. Eng.	66	319	1988
518	J. Chem. Eng. Data	38	386	1993
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522	J. Supercritical Fluids	8	205	1995
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524	J. Chem. Eng. Data	35	63	1990
525	J. Chem. Eng. Japan	28	263	1995

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528	Fluid Phase Equilibria	36	235	1987
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530	Fluid Phase Equilibria	26	165	1986
531	J. Chem. Thermodyamics	29	197	1997
532	J. Chem. Eng. Data	35	278	1990
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538	Ind. Eng. Chem. Res.	33	1955	1994
539	Fluid Phase Equilibria	73	117	1992
540	J. Chem. Eng. Data	37	213	1992
541	J. Chem. Eng. Japan	25	211	1992
542	J. Chem. Eng. Japan	21	25	1988
543	J. Chem. Eng. Data	20	264	1975
544	J. Chem. Eng. Data	38	53	1993
545	J. Supercritical Fluids	13	23	1998
546	J. Chem. Eng. Data	41	339	1996
547	J. Chem. Eng. Data	42	155	1997
548	J. Chem. Eng. Data	40	850	1995
549	Fluid Phase Equilibria	112	125	1995
550	Fluid Phase Equilibria	157	285	1999
551	Fluid Phase Equilibria	141	179	1997
552	J. Chem. Eng. Data	36	80	1991
553	J. Chem. Eng. Data	28	52	1983
554	J. Chem. Eng. Data	31	26	1986
555	J. Chem. Eng. Data	30	259	1985
556	J. Chem. Eng. Data	31	43	1986
557	J. Chem. Eng. Data	26	155	1981
558	J. Chem. Eng. Data	34	324	1989
559	Ind. Eng. Chem.	41	2039	1949
560	J. Chem. Eng. Data	8	14	1963
561	J. Chem. Eng. Data	27	281	1982
562	J. Chem. Eng. Data	41	1239	1996
563	J. Chem. Thermodynamics	35	1567	2003
564	J. Chem. Eng. Data	34	409	1989
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566	Fluid Phase Equilibria	212	81	2003
567	Fluid Phase Equilibria	212	129	2003
568	Thermochimica Acta	306	85	1997
569	Fluid Phase Equilibria	134	163	1997
570	J. Chem. Eng. Data	42	132	1997
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572	J. Chem. Eng. Data	34	270	1989
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574	J. Chem. Eng. Data	5	416	1960
575	J. Chem. Eng. Data	13	301	1968
576	J. Chem. Eng. Data	46	1410	2001
577	J. Chem. Eng. Data	40	515	1995

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579	J. Chem. Eng. Data	34	391	1989
580	J. Chem. Eng. Data	30	455	1985
581	J. Chem. Eng. Data	44	303	1999
582	J. Chem. Eng. Data	43	941	1998
583	Int. Data Ser., Selec. Data Mixtures, Ser. A		194	1996
584	Int. Data Ser., Selec. Data Mixtures, Ser. A		180	1996
585	J. Soln. Chem.	24	357	1995
586	Int. Data Ser., Selec. Data Mixtures, Ser. A		95	1975
587	J. Chem. Thermodynamics	21	731	1989
588	J. Chem. Eng. Data	38	274	1993
589	J. Chem. Eng. Data	28	30	1983
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591	J. Chem. Thermodynamics	18	81	1986

APPENDIX F

EXPERIMENTAL SOLID SOLUBILITY DATA WITH MOSCED AND UNIFAC PREDICTIONS

Table F-1. Solubility of 2-Hydroxybenzoic acid in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Sharp et al. 1999).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
1-propanol	298.15	0.1636	0.0867	0.1346	18%	0.1260	23%
2-propanol	298.15	0.1789	0.0867	0.1267	29%	0.1674	6%
1-butanol	298.15	0.1646	0.0867	0.1141	31%	0.1666	1%
2-butanol	298.15	0.1869	0.0867	0.1141	39%	0.1537	18%
2-methyl-1-propanol	298.15	0.1430	0.0867	0.1141	20%	0.1595	12%
2-methyl-2-propanol	298.15	0.2193	0.0867	0.0821	63%	0.2125	3%
1-pentanol	298.15	0.1611	0.0867	0.0981	39%	0.1418	12%
1-octanol	298.15	0.2143	0.0867	0.0676	68%	0.1948	9%
dibutyl ether	298.15	0.0919	0.0867	0.0154	83%	0.0925	1%
1,4-dioxane	298.15	0.2945	0.0867			0.2262	23%
tetrahydrofuran	298.15	0.3642	0.0867			0.3724	2%
2-butanone	298.15	0.1852	0.0867	0.2606	41%	0.2254	22%
cyclohexanone	298.15	0.2301	0.0867	0.2222	3%	0.2848	24%
ethyl acetate	298.15	0.1425	0.0867	0.1815	27%	0.2470	73%
butyl acetate	298.15	0.1363	0.0867	0.2111	55%	0.2254	65%
acetone	298.15	0.1817	0.0867	0.2852	57%	0.2303	27%

Table F-2. Solubility of 2-Nitro-5-methylphenol in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Buchowski, Domanska et al. 1975).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
Methanol	298.15	0.0535	0.4774			0.0401	25%
Ethanol	298.15	0.0426	0.4774			0.0516	21%
1-Propanol	298.15	0.0525	0.4774			0.0525	0%
1-Butanol	298.15	0.0630	0.4774			0.0757	20%
1-Hexanol	298.15	0.0868	0.4774			0.0665	23%
1-Octanol	298.15	0.1018	0.4774			0.0906	11%
Ethyl acetate	298.15	0.4354	0.4774			0.4621	6%
Butyl acetate	298.15	0.4336	0.4774			0.4343	0%
Carbon tetrachloride	298.15	0.3699	0.4774			0.3062	17%
Benzene	298.15	0.4189	0.4774			0.4486	7%
Cyclohexane	298.15	0.0540	0.4774			0.0774	43%
Hexane	298.15	0.0414	0.4774			0.0414	0%
Decane	298.15	0.0726	0.4774			0.0469	35%
Hexadecane	298.15	0.0942	0.4774			0.0547	42%
Acetone	298.15	0.4464	0.4774			0.4874	9%
m-Cresol	298.15	0.3989	0.4774			0.3989	0%
Nitrobenzene	298.15	0.4915	0.4774			0.4721	4%

Table F-3. Solubility of 4-Nitro-5-methylphenol in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Buchowski, Jodzewicz et al. 1975).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
Benzene	298.15	0.003748	0.0834			0.0061	62%
Dibutyl ether	298.15	0.055515	0.0834			0.0639	15%
Nitrobenzene	298.15	0.056422	0.0834			0.0331	41%
Dipropyl ether	298.15	0.139067	0.0834			0.0680	51%
1-Octanol	298.15	0.180922	0.0834			0.1829	1%
1-Pentanol	298.15	0.18848	0.0834			0.1005	47%
1-Butanol	298.15	0.189362	0.0834			0.1331	30%
1-Propanol	298.15	0.189504	0.0834			0.0872	54%
Ethanol	298.15	0.203028	0.0834			0.1400	31%
Butyl acetate	298.15	0.204743	0.0834			0.2771	35%
Pentyl acetate	298.15	0.208176	0.0834			0.2022	3%
Ethyl acetate	298.15	0.22768	0.0834			0.3360	48%
Methyl isobutyl ketone	298.15	0.262853	0.0834			0.2658	1%
2-Butanone	298.15	0.298775	0.0834			0.5647	89%
Methanol	298.15	0.304976	0.0834			0.1277	58%
Acetone	298.15	0.312674	0.0834			0.5413	73%
1-Hexanol	298.15	0.185929	0.0834			0.0894	52%
m-Cresol	298.15	0.068222	0.0834			0.0709	4%
water	298.15	0.00014	0.0834			0.0002	16%

Table F-4. Solubility of Acenaphthene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Sharp et al. 1999).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.051920	0.20044	0.05295	2%	0.05806	12%
heptane	298.15	0.060750	0.20044	0.05942	2%	0.06336	4%
octane	298.15	0.068260	0.20044	0.06480	5%	0.06715	2%
nonane	298.15	0.072100	0.20044	0.06947	4%	0.07148	1%
decane	298.15	0.078520	0.20044	0.07364	6%	0.07413	6%
hexadecane	298.15	0.106500	0.20044	0.09334	12%	0.09282	13%
cyclohexane	298.15	0.070430	0.20044	0.08263	17%	0.10154	44%
methylcyclohexane	298.15	0.080930	0.20044	0.08418	4%	0.08351	3%
cyclooctane	298.15	0.097390	0.20044	0.07728	21%	0.10270	5%
2,2,4-trimethylpentane	298.15	0.046680	0.20044	0.06500	39%	0.04006	14%
dibutyl ether	298.15	0.111600	0.20044	0.11096	1%	0.10224	8%
tetrahydrofuran	298.15	0.197300	0.20044	0.19470	1%	0.18069	8%
dioxane	298.15	0.141500	0.20044	0.14526	3%	0.18258	29%
methanol	298.15	0.005440	0.20044	0.01062	95%	0.00639	17%
ethanol	298.15	0.010680	0.20044	0.01539	44%	0.01139	7%
1-propanol	298.15	0.016860	0.20044	0.02441	45%	0.01830	9%
2-propanol	298.15	0.013360	0.20044	0.02278	71%	0.01551	16%
1-butanol	298.15	0.023730	0.20044	0.03238	36%	0.02476	4%
2-butanol	298.15	0.018770	0.20044	0.03238	73%	0.02360	26%
2-methyl-1-propanol	298.15	0.016910	0.20044	0.03238	91%	0.02043	21%
2-methyl-2-propanol	298.15	0.017050	0.20044	0.01931	13%	0.03065	80%
1-pentanol	298.15	0.031760	0.20044	0.03939	24%	0.03065	3%
1-hexanol	298.15	0.039220	0.20044	0.04562	16%	0.02865	27%
1-octanol	298.15	0.050890	0.20044	0.05638	11%	0.03852	24%
2-butanone	298.15	0.130700	0.20044	0.11858	9%	0.11839	9%
butyl acetate	298.15	0.137000	0.20044	0.14072	3%	0.13786	1%
ethyl acetate	298.15	0.108600	0.20044	0.07902	27%	0.11389	5%
tert-butylcyclohexane	298.15	0.077630	0.20044	0.09095	17%		
2-pentanol	298.15	0.024430	0.20044	0.02268	7%		
3-methyl-1-butanol	298.15	0.023470	0.20044	0.02701	15%		
2-methyl-2-butanol	298.15	0.028670	0.20044	0.03942	37%		
2-methyl-1-pentanol	298.15	0.029040	0.20044	0.04562	57%		
4-methyl-2-pentanol	298.15	0.025510	0.20044	0.04307	69%		
1-heptanol	298.15	0.046170	0.20044	0.04562	1%		
2-ethyl-1-hexanol	298.15	0.044020	0.20044	0.05638	28%		
ethylene glycol	298.15	0.001157	0.20044	0.00044	62%		

Table F-5. Solubility of Acetaminophen in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Granberg and Rasmuson 1999).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
water	303.15	0.002068	0.08938			0.00173	16%
methanol	303.15	0.073020	0.08938			0.05724	22%
ethanol	303.15	0.066237	0.08938			0.05270	20%
1,2-ethanediol	303.15	0.055937	0.08938				
1-propanol	303.15	0.050138	0.08938			0.04892	2%
2-propanol	303.15	0.050941	0.08938			0.03753	26%
1-butanol	303.15	0.043901	0.08938			0.04390	0%
1-pentanol	303.15	0.038045	0.08938			0.03954	4%
1-hexanol	303.15	0.032509	0.08938			0.03346	3%
1-heptanol	303.15	0.027969	0.08938				
1-octanol	303.15	0.023119	0.08938			0.02353	2%
acetone	303.15	0.041134	0.08938			0.00937	77%
2-butanone	303.15	0.032308	0.08938			0.00767	76%
4-methyl-2-pentanone	303.15	0.011664	0.08938			0.00124	89%
tetrahydrofuran	303.15	0.069001	0.08938			0.01519	78%
1,4-dioxane	303.15	0.009857	0.08938			0.01816	84%
ethyl acetate	303.15	0.006215	0.08938			0.00194	69%
acetonitrile	303.15	0.008837	0.08938			0.00552	38%
diethylamine	303.15	0.389192	0.08938				
N,N-dimethylformamide	303.15	0.328576	0.08938			0.20633	37%
dimethyl sulfoxide	303.15	0.369254	0.08938			0.33955	8%
acetic acid	303.15	0.031817	0.08938			0.09581	
dichloromethane	303.15	0.000180	0.08938			0.00062	
chloroform	303.15	0.001215	0.08938			0.00051	
carbon tetrachloride	303.15	0.000905	0.08938			0.00002	
toluene	303.15	0.000207	0.08938			0.00012	43%

Table F-6. Solubility of Anthracene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Hansen, Riverol et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.001290	0.01025	0.00120	7%	0.00141	9%
heptane	298.15	0.001571	0.01025	0.00139	12%	0.00156	0%
octane	298.15	0.001850	0.01025	0.00155	16%	0.00167	10%
decane	298.15	0.002345	0.01025	0.00182	22%	0.00185	21%
hexadecane	298.15	0.003800	0.01025	0.00246	35%	0.00233	39%
2,2,4-trimethylpentane	298.15	0.001087	0.01025	0.00155	43%	0.00088	19%
cyclohexane	298.15	0.001574	0.01025	0.00181	15%	0.00280	78%
methylcyclohexane	298.15	0.001650	0.01025	0.00190	15%	0.00221	34%
cyclooctane	298.15	0.002258	0.01025	0.00178	21%	0.00281	24%
benzene	298.15	0.007418	0.01025	0.00946	28%	0.01098	48%
toluene	298.15	0.007360	0.01025	0.00925	26%	0.00891	21%
m-xylene	298.15	0.007956	0.01025	0.00878	10%		
p-xylene	298.15	0.007330	0.01025	0.00878	20%	0.00682	7%
methanol	298.15	0.000243	0.01025	0.00033	34%	0.00013	47%
ethanol	298.15	0.000460	0.01025	0.00037	20%	0.00025	46%
1-propanol	298.15	0.000591	0.01025	0.00059	1%	0.00042	29%
2-propanol	298.15	0.000411	0.01025	0.00055	33%	0.00035	15%
1-butanol	298.15	0.000801	0.01025	0.00080	0%	0.00061	24%
2-butanol	298.15	0.000585	0.01025	0.00080	37%	0.00057	3%
2-methyl-1-propanol	298.15	0.000470	0.01025	0.00080	71%	0.00048	2%
1-pentanol	298.15	0.001097	0.01025	0.00099	9%	0.00076	31%
1-hexanol	298.15	0.001483	0.01025	0.00117	21%	0.00067	55%
1-heptanol	298.15	0.001869	0.01025	0.00117	37%		
1-octanol	298.15	0.002160	0.01025	0.00148	32%	0.00092	57%
acetone	298.15	0.003100	0.01025	0.00441	42%	0.00275	11%
2-butanone	298.15	0.004770	0.01025	0.00529	11%	0.00528	11%
diethyl ether	298.15	0.002900	0.01025	0.00289	0%	0.00290	0%
dibutyl ether	298.15	0.003540	0.01025	0.00364	3%	0.00330	7%
dioxane	298.15	0.008381	0.01025	0.00563	33%	0.01097	31%
ethyl acetate	298.15	0.004840	0.01025	0.00327	32%	0.00485	0%
butyl acetate	298.15	0.006610	0.01025	0.00628	5%	0.00598	10%
diethyl adipate	298.15	0.010330	0.01025	0.00654	37%		
dichloromethane	298.15	0.009387	0.01025	0.00451	52%	0.01374	46%
chloroform	298.15	0.010840	0.01025	0.01291	19%	0.01441	33%
carbon tetrachloride	298.15	0.004640	0.01025	0.00522	13%	0.00692	49%
1-chlorobutane	298.15	0.005860	0.01025	0.00371	37%	0.00680	16%
1,4-dichlorobutane	298.15	0.010530	0.01025	0.00649	38%		
1-chlorooctane	298.15	0.007780	0.01025	0.00423	46%		
chlorocyclohexane	298.15	0.006353	0.01025	0.00576	9%		
chlorobenzene	298.15	0.009962	0.01025	0.01312	32%	0.01054	6%
ethylene glycol	298.15	0.000072	0.01025	0.00001	82%		
acetonitrile	298.15	0.000830	0.01025	0.00280	237%	0.00099	19%
N,N-dimethylformamide	298.15	0.007839	0.01025	0.00532	32%	0.00269	66%

Table F-7. Solubility of Benzil in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fletcher, Pandey et al. 1995).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.005700	0.22381	0.00995	74%	0.00584	2%
heptane	298.15	0.006590	0.22381	0.01186	80%	0.00667	1%
octane	298.15	0.007260	0.22381	0.01350	86%	0.00723	0%
nonane	298.15	0.007940	0.22381	0.01493	88%	0.00789	1%
cyclohexane	298.15	0.010680	0.22381	0.02076	94%	0.01665	56%
methylcyclohexane	298.15	0.011280	0.22381	0.02137	89%	0.01101	2%
cyclooctane	298.15	0.014540	0.22381	0.01844	27%	0.01708	17%
2,2,4-trimethylpentane	298.15	0.005870	0.22381	0.01356	131%	0.00315	46%
benzene	298.15	0.180400	0.22381	0.23234	29%	0.19289	7%
toluene	298.15	0.150400	0.22381	0.21802	45%	0.14894	1%
carbon tetrachloride	298.15	0.080820	0.22381	0.19741	144%	0.09121	13%
1-chlorobutane	298.15	0.104700	0.22381	0.06417	39%	0.08381	20%
1,2-dichloroethane	298.15	0.226400	0.22381	0.32487	43%	0.23236	3%
dibutyl ether	298.15	0.033510	0.22381	0.04342	30%	0.03784	13%
tetrahydrofuran	298.15	0.251200	0.22381	0.20916	17%	0.24727	2%
1,4-dioxane	298.15	0.210100	0.22381	0.22546	7%	0.27609	31%
ethyl acetate	298.15	0.145500	0.22381	0.13132	10%	0.13210	9%
butyl acetate	298.15	0.135000	0.22381	0.15848	17%	0.12323	9%
methanol	298.15	0.007830	0.22381	0.02305	194%	0.00513	35%
ethanol	298.15	0.010310	0.22381	0.01611	56%	0.00702	32%
1-propanol	298.15	0.011840	0.22381	0.02159	82%	0.00965	19%
2-propanol	298.15	0.008310	0.22381	0.01817	119%	0.00707	15%
1-butanol	298.15	0.013060	0.22381	0.02526	93%	0.01294	1%
2-butanol	298.15	0.011030	0.22381	0.02526	129%	0.01064	4%
2-methyl-1-propanol	298.15	0.009690	0.22381	0.02526	161%	0.00913	6%
1-pentanol	298.15	0.015030	0.22381	0.02791	86%	0.01517	1%
1-hexanol	298.15	0.015630	0.22381	0.02995	92%	0.01217	22%
1-octanol	298.15	0.016920	0.22381	0.03306	95%	0.01600	5%
cyclopentanol	298.15	0.017920	0.22381	0.03419	91%		
tert-butylcyclohexane	298.15	0.011140	0.22381	0.02358	112%		
1-heptanol	298.15	0.016430	0.22381	0.02995	82%		
2-pentanol	298.15	0.012740	0.22381	0.01214	5%		
3-methyl-1-butanol	298.15	0.012140	0.22381	0.01640	35%		
2-methyl-2-butanol	298.15	0.016730	0.22381	0.02797	67%		
4-methyl-2-pentanol	298.15	0.012820	0.22381	0.02631	105%		
2-ethyl-1-hexanol	298.15	0.015630	0.22381	0.03306	112%		

Table F-8. Solubility of Biphenyl in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Sharp et al. 1999).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.124	0.3987	0.1405	13%	0.1482	20%
heptane	298.15	0.138	0.3987	0.1471	7%	0.1495	8%
octane	298.15	0.147	0.3987	0.1524	4%	0.1493	2%
nonane	298.15	0.1551	0.3987	0.1570	1%	0.1511	3%
decane	298.15	0.1636	0.3987	0.1613	1%	0.1512	8%
hexadecane	298.15	0.2151	0.3987	0.1833	15%	0.1650	23%
cyclohexane	298.15	0.19	0.3987	0.1969	4%	0.2421	27%
methylcyclohexane	298.15	0.183	0.3987	0.1949	6%	0.1963	7%
cyclooctane	298.15	0.2194	0.3987	0.1687	23%	0.2060	6%
2,2,4-trimethylpentane	298.15	0.1094	0.3987	0.1528	40%	0.0968	11%
benzene	298.15	0.381	0.3987	0.4082	7%	0.4020	6%
toluene	298.15	0.377	0.3987	0.4014	6%	0.3837	2%
ethylbenzene	298.15	0.363	0.3987	0.3686	2%	0.3780	4%
chlorobenzene	298.15	0.397	0.3987	0.4160	5%	0.4019	1%
dichloromethane	298.15	0.412	0.3987	0.3992	3%	0.4184	2%
1,2-dichloroethane	298.15	0.397	0.3987	0.4338	9%	0.3992	1%
1,1-dichloroethane	298.15	0.381	0.3987	0.3922	3%	0.3922	3%
chloroform	298.15	0.422	0.3987	0.4323	2%	0.4109	3%
carbon tetrachloride	298.15	0.342	0.3987	0.3643	7%	0.3574	5%
dibutyl ether	298.15	0.266	0.3987	0.2734	3%	0.2556	4%
methanol	298.15	0.01851	0.3987	0.0242	30%	0.0134	27%
ethanol	298.15	0.03456	0.3987	0.0258	25%	0.0251	27%
1-propanol	298.15	0.0462	0.3987	0.0430	7%	0.0363	22%
2-propanol	298.15	0.03533	0.3987	0.0433	23%	0.0364	3%
1-butanol	298.15	0.05788	0.3987	0.0584	1%	0.0535	8%
2-butanol	298.15	0.05005	0.3987	0.0584	17%	0.0520	4%
2-methyl-1-propanol	298.15	0.03906	0.3987	0.0584	50%	0.0468	20%
2-methyl-2-propanol	298.15	0.04118	0.3987	0.0432	5%	0.0758	84%
1-pentanol	298.15	0.07573	0.3987	0.0718	5%	0.0612	19%
1-hexanol	298.15	0.08592	0.3987	0.0835	3%	0.0571	34%
1-octanol	298.15	0.1097	0.3987	0.1033	6%	0.0787	28%
carbon disulfide	298.15	0.369	0.3987	0.3916	6%	0.3843	4%
tert-butylcyclohexane	298.15	0.174	0.3987	0.1877	8%		
2-pentanol	298.15	0.06525	0.3987	0.0492	25%		
3-methyl-1-butanol	298.15	0.05664	0.3987	0.0550	3%		
2-methyl-2-butanol	298.15	0.0712	0.3987	0.0718	1%		
2-methyl-1-pentanol	298.15	0.07216	0.3987	0.0835	16%		
4-methyl-2-pentanol	298.15	0.06115	0.3987	0.0825	35%		
1-heptanol	298.15	0.1001	0.3987	0.0835	17%		
2-ethyl-1-hexanol	298.15	0.09481	0.3987	0.1033	9%		
ethylene glycol	298.15	0.00269	0.3987	0.0010	61%		
1,2-dibromoethane	298.15	0.389	0.3987	0.3584	8%		

Table F-9. Solubility of Diphenyl sulfone in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Van et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.000524	0.10997			0.00071	35%
heptane	298.15	0.000593	0.10997			0.00075	26%
octane	298.15	0.000672	0.10997			0.00077	15%
nonane	298.15	0.000745	0.10997			0.00080	7%
decane	298.15	0.000819	0.10997			0.00081	1%
hexadecane	298.15	0.001411	0.10997			0.00092	35%
cyclohexane	298.15	0.000872	0.10997			0.00094	8%
methylcyclohexane	298.15	0.000882	0.10997			0.00087	2%
cyclooctane	298.15	0.00126	0.10997			0.00086	32%
2,2,4-trimethylpentane	298.15	0.000497	0.10997			0.00054	9%
squalane	298.15	0.00194	0.10997			0.00082	58%
1,2-dichloroethane	298.15	0.1093	0.10997			0.15201	39%
1-chlorobutane	298.15	0.02253	0.10997			0.02014	11%
dibutyl ether	298.15	0.00414	0.10997			0.00383	7%
methyl tert-butyl ether	298.15	0.00932	0.10997			0.00807	13%
tetrahydrofuran	298.15	0.1051	0.10997			0.04884	54%
1,4-dioxane	298.15	0.0902	0.10997			0.10027	11%
methanol	298.15	0.00491	0.10997			0.00649	32%
ethanol	298.15	0.00535	0.10997			0.00478	11%
1-propanol	298.15	0.00527	0.10997			0.00400	24%
2-propanol	298.15	0.00349	0.10997			0.00350	0%
1-butanol	298.15	0.00527	0.10997			0.00440	16%
2-butanol	298.15	0.00436	0.10997			0.00355	19%
2-methyl-1-propanol	298.15	0.00397	0.10997			0.00383	4%
2-methyl-2-propanol	298.15	0.00423	0.10997			0.00598	41%
1-pentanol	298.15	0.00532	0.10997			0.00403	24%
1-hexanol	298.15	0.00528	0.10997			0.00324	39%
1-octanol	298.15	0.00484	0.10997			0.00282	42%
1-decanol	298.15	0.00466	0.10997			0.00544	17%
butyl acetate	298.15	0.0341	0.10997			0.02828	17%
ethyl acetate	298.15	0.04458	0.10997			0.05636	26%
methyl acetate	298.15	0.04978	0.10997			0.06991	40%
cyclopentanol	298.15	0.00943	0.10997				
tert-butylcyclohexane	298.15	0.00114	0.10997				
1-chlorooctane	298.15	0.01183	0.10997				
chlorocyclohexane	298.15	0.02541	0.10997				
2-pentanol	298.15	0.00453	0.10997				
3-methyl-1-butanol	298.15	0.00453	0.10997				
2-methyl-2-butanol	298.15	0.0055	0.10997				
2-methyl-1-pentanol	298.15	0.00449	0.10997				
4-methyl-2-pentanol	298.15	0.0045	0.10997				
1-heptanol	298.15	0.00498	0.10997				
2-ethyl-1-hexanol	298.15	0.005304	0.10997				

Table F-10. Solubility of Diuron in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Sharp et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.00001828	0.01521			3.11E-05	70%
heptane	298.15	0.00002703	0.01521			3.31E-05	23%
octane	298.15	0.00002934	0.01521			3.45E-05	18%
nonane	298.15	0.00003615	0.01521			3.59E-05	1%
decane	298.15	0.00004192	0.01521			3.68E-05	12%
hexadecane	298.15	0.00006794	0.01521			4.23E-05	38%
cyclohexane	298.15	0.00002676	0.01521			4.31E-05	61%
methylcyclohexane	298.15	0.00004661	0.01521			3.93E-05	16%
cyclooctane	298.15	0.00006082	0.01521			4.09E-05	33%
2,2,4-trimethylpentane	298.15	0.00002694	0.01521			2.32E-05	14%
benzene	298.15	0.0008417	0.01521			6.48E-04	23%
toluene	298.15	0.0008907	0.01521			5.08E-04	43%
ethylbenzene	298.15	0.00072	0.01521			3.20E-04	55%
chlorobenzene	298.15	0.001686	0.01521			5.12E-04	70%
dichloromethane	298.15	0.002922	0.01521			3.29E-03	12%
1,2-dichloroethane	298.15	0.004258	0.01521			1.61E-03	62%
chloroform	298.15	0.005354	0.01521			5.31E-03	1%
carbon tetrachloride	298.15	0.0002389	0.01521			2.59E-04	9%
1-chlorobutane	298.15	0.001086	0.01521			2.31E-04	79%
dibutyl ether	298.15	0.005037	0.01521			9.04E-04	82%
tetrahydrofuran	298.15	0.0306	0.01521			2.05E-02	33%
1,4-dioxane	298.15	0.007188	0.01521			1.67E-02	133%
methanol	298.15	0.007681	0.01521			9.35E-03	22%
ethanol	298.15	0.009406	0.01521			9.64E-03	2%
1-propanol	298.15	0.01068	0.01521			1.03E-02	4%
2-propanol	298.15	0.0077	0.01521			8.01E-03	4%
1-butanol	298.15	0.01197	0.01521			1.00E-02	16%
2-butanol	298.15	0.008521	0.01521			8.61E-03	1%
2-methyl-1-propanol	298.15	0.008479	0.01521			8.17E-03	4%
2-methyl-2-propanol	298.15	0.006467	0.01521			1.11E-02	71%
1-pentanol	298.15	0.01402	0.01521			9.77E-03	30%
1-hexanol	298.15	0.01442	0.01521			8.43E-03	42%
1-octanol	298.15	0.01581	0.01521			7.81E-03	51%
1-decanol	298.15	0.01397	0.01521			7.25E-03	48%
butyl acetate	298.15	0.009931	0.01521			2.66E-03	73%
ethyl acetate	298.15	0.009135	0.01521			3.61E-03	60%
acetonitrile	298.15	0.004296	0.01521			3.07E-03	28%
tert-butylcyclohexane	298.15	0.00007557	0.01521				
1-chlorooctane	298.15	0.00198	0.01521				
chlorocyclohexane	298.15	0.001427	0.01521				
2-pentanol	298.15	0.009004	0.01521				
3-methyl-1-butanol	298.15	0.01073	0.01521				
2-methyl-2-butanol	298.15	0.005469	0.01521				
2-methyl-1-pentanol	298.15	0.01122	0.01521				
4-methyl-2-pentanol	298.15	0.007564	0.01521				
1-heptanol	298.15	0.01506	0.01521				
2-ethyl-1-hexanol	298.15	0.009674	0.01521				
cyclopentanol	298.15	0.01437	0.01521				
ethylene glycol	298.15	9.565E-08	0.01521				

Table F-11. Solubility of Fluoranthene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Hansen, Riverol et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.01476	0.21479	0.01381	6%	0.00820	44%
heptane	298.15	0.01870	0.21479	0.01660	11%	0.00981	48%
octane	298.15	0.02260	0.21479	0.01904	16%	0.01099	51%
nonane	298.15	0.02642	0.21479	0.02121	20%	0.01238	53%
decane	298.15	0.03015	0.21479	0.02316	23%	0.01312	56%
hexadecane	298.15	0.05046	0.21479	0.03241	36%	0.01863	63%
methylcyclohexane	298.15	0.02179	0.21479	0.02771	27%	0.01871	14%
cyclooctane	298.15	0.03011	0.21479	0.02423	20%	0.03623	20%
2,2,4-trimethylpentane	298.15	0.01162	0.21479	0.01913	65%	0.00387	67%
benzene	298.15	0.12110	0.21479	0.19733	63%	0.17069	41%
toluene	298.15	0.11600	0.21479	0.18913	63%	0.13709	18%
methanol	298.15	0.00267	0.21479	0.00504	89%	0.00222	17%
ethanol	298.15	0.00544	0.21479	0.00577	6%	0.00387	29%
1-propanol	298.15	0.00670	0.21479	0.00948	41%	0.00669	0%
2-propanol	298.15	0.00475	0.21479	0.00791	67%	0.00438	8%
1-butanol	298.15	0.00996	0.21479	0.01282	29%	0.00948	5%
2-butanol	298.15	0.00702	0.21479	0.01282	83%	0.00785	12%
2-methyl-1-propanol	298.15	0.00495	0.21479	0.01282	159%	0.00605	22%
1-pentanol	298.15	0.01446	0.21479	0.01578	9%	0.01260	13%
1-hexanol	298.15	0.01986	0.21479	0.01841	7%	0.01026	48%
1-octanol	298.15	0.03125	0.21479	0.02296	27%	0.01645	47%
dibutyl ether	298.15	0.05177	0.21479	0.05042	3%	0.05180	0%
ethyl acetate	298.15	0.08589	0.21479	0.04997	42%	0.08597	0%
butyl acetate	298.15	0.11060	0.21479	0.11934	8%	0.10929	1%
carbon tetrachloride	298.15	0.08157	0.21479	0.10836	33%	0.09630	18%
chloroform	298.15	0.14200	0.21479	0.22454	58%	0.16520	16%
1,2-dichloroethane	298.15	0.12680	0.21479	0.18300	44%	0.16301	29%
1-chlorobutane	298.15	0.11330	0.21479	0.05613	50%	0.06583	42%
N,N-dimethylacetamide	298.15	0.23700	0.21479	0.21463	9%	0.25816	9%
N,N-dimethylformamide	298.15	0.17970	0.21479	0.13752	23%	0.16827	6%
acetonitrile	298.15	0.01315	0.21479	0.08645	557%	0.01031	22%
cyclohexane	298.15	0.01807	0.21479	0.02650	47%	0.03176	76%
tert-butylcyclohexane	298.15	0.02482	0.21479	0.03201	29%		
2-pentanol	298.15	0.01021	0.21479	0.00651	36%		
3-methyl-1-butanol	298.15	0.00862	0.21479	0.00866	0%		
2-methyl-2-butanol	298.15	0.00970	0.21479	0.01581	63%		
2-methyl-1-pentanol	298.15	0.01172	0.21479	0.01841	57%		
4-methyl-2-pentanol	298.15	0.00948	0.21479	0.01617	71%		
1-heptanol	298.15	0.02524	0.21479	0.01841	27%		
2-ethyl-1-hexanol	298.15	0.01782	0.21479	0.02296	29%		
ethylene glycol	298.15	0.00075	0.21479	0.00013	83%		
cyclopentanol	298.15	0.01772	0.21479	0.01795	1%		
1-chlorohexane	298.15	0.13150	0.21479	0.06178	53%		
1-chlorooctane	298.15	0.13670	0.21479	0.06255	54%		
chlorocyclohexane	298.15	0.11590	0.21479	0.10246	12%		

Table F-12. Solubility of Hexachlorobenzene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Van et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.002620	0.01534	0.52448	19918%	0.00282	8%
heptane	298.15	0.003140	0.01534	0.56206	17800%	0.00332	6%
octane	298.15	0.003710	0.01534	0.59175	15850%	0.00370	0%
nonane	298.15	0.004100	0.01534	0.61644	14935%	0.00414	1%
decane	298.15	0.004600	0.01534	0.63757	13760%	0.00440	4%
hexadecane	298.15	0.006810	0.01534	0.72219	10505%	0.00628	8%
cyclohexane	298.15	0.002950	0.01534	0.64558	21784%	0.00767	160%
methylcyclohexane	298.15	0.003870	0.01534	0.65191	16745%	0.00539	39%
2,2,4-trimethylpentane	298.15	0.002520	0.01534	0.59263	23417%	0.00157	38%
tert-butylcyclohexane	298.15	0.004710	0.01534	0.69926	14746%		
1,2-dichloroethane	298.15	0.002860	0.01534	0.60489	21050%	0.00514	80%
1-chlorobutane	298.15	0.003830	0.01534	0.51309	13297%	0.00509	33%
1-chlorohexane	298.15	0.005080	0.01534	0.59107	11535%		
1-chlorooctane	298.15	0.006060	0.01534	0.64321	10514%		
chlorocyclohexane	298.15	0.006100	0.01534	0.66490	10800%		
dibutyl ether	298.15	0.004400	0.01534	0.75335	17022%	0.00399	9%
methyl tert-butyl ether	298.15	0.003200	0.01534	0.74296	23117%	0.00433	35%
tetrahydrofuran	298.15	0.005920	0.01534	0.46087	7685%	0.00612	3%
1,4-dioxane	298.15	0.003970	0.01534	0.01055	166%	0.00603	52%
methanol	298.15	0.000090	0.01534	0.01003	11022%	0.00008	17%
ethanol	298.15	0.000236	0.01534	0.33461	141684%	0.00018	25%
1-propanol	298.15	0.000398	0.01534	0.41076	103105%	0.00041	3%
2-propanol	298.15	0.000298	0.01534	0.37206	124752%	0.00027	9%
1-butanol	298.15	0.000667	0.01534	0.46821	70096%	0.00056	16%
2-butanol	298.15	0.000521	0.01534	0.46821	89767%	0.00053	2%
2-methyl-1-propanol	298.15	0.000533	0.01534	0.46821	87744%	0.00040	26%
2-methyl-2-propanol	298.15	0.000517	0.01534	0.21942	42341%	0.00063	21%
1-pentanol	298.15	0.001030	0.01534	0.51356	49760%	0.00083	19%
2-pentanol	298.15	0.000860	0.01534	0.27924	32370%		
3-methyl-1-butanol	298.15	0.000770	0.01534	0.38103	49385%		
2-methyl-2-butanol	298.15	0.001200	0.01534	0.51389	42725%		
1-hexanol	298.15	0.001440	0.01534	0.55052	38131%	0.00075	48%
2-methyl-1-pentanol	298.15	0.001400	0.01534	0.55052	39223%		
4-methyl-2-pentanol	298.15	0.001430	0.01534	0.52421	36558%		
1-heptanol	298.15	0.001900	0.01534	0.55052	28875%		
1-octanol	298.15	0.002380	0.01534	0.60759	25429%	0.00113	53%
2-ethyl-1-hexanol	298.15	0.001740	0.01534	0.60759	34819%		
1-decanol	298.15	0.003800	0.01534	0.64996	17004%	0.00328	14%
cyclopentanol	298.15	0.000920	0.01534	0.55447	60168%		
butyl acetate	298.15	0.003650	0.01534	0.64674	17619%	0.00362	1%
ethyl acetate	298.15	0.002110	0.01534	0.64003	30233%	0.00191	10%
methyl acetate	298.15	0.001480	0.01534	0.60579	40832%	0.00075	50%

Table F-13. Solubility of Ibuprofen in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Gracin and Rasmuson 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
methanol	283.15	0.101312	0.14917	0.07107	30%	0.08782	13%
ethanol	283.15	0.116881	0.14917	0.05127	56%	0.12832	10%
2-propanol	283.15	0.128320	0.14917	0.07239	44%	0.15269	19%
acetone	283.15	0.141958	0.14917	0.15118	6%	0.21034	48%
methyl isobutyl ketone	283.15	0.132770	0.14917	0.16384	23%	0.16538	25%
chloroform	283.15	0.209337	0.14917	0.25617	22%	0.14321	32%
ethyl acetate	283.15	0.122617	0.14917	0.10563	14%	0.18345	50%
toluene	283.15	0.103442	0.14917	0.12956	25%	0.07656	26%
methanol	288.15	0.125304	0.17601	0.09352	25%	0.10834	14%
ethanol	288.15	0.146052	0.17601	0.06435	56%	0.15449	6%
2-propanol	288.15	0.161024	0.17601	0.08942	44%	0.18211	13%
acetone	288.15	0.167364	0.17601	0.18084	8%	0.23868	43%
methyl isobutyl ketone	288.15	0.159526	0.17601	0.19206	20%	0.19340	21%
chloroform	288.15	0.242938	0.17601	0.28475	17%	0.17689	27%
ethyl acetate	288.15	0.150505	0.17601	0.13221	12%	0.21201	41%
toluene	288.15	0.132889	0.17601	0.15721	18%	0.10476	21%
methanol	293.15	0.138495	0.20687	0.12314	11%	0.13383	3%
ethanol	293.15	0.165267	0.20687	0.08242	50%	0.18521	12%
2-propanol	293.15	0.187837	0.20687	0.11187	40%	0.21555	15%
acetone	293.15	0.199168	0.20687	0.21477	8%	0.26998	36%
methyl isobutyl ketone	293.15	0.191466	0.20687	0.22415	17%	0.22518	18%
chloroform	293.15	0.271750	0.20687	0.31592	16%	0.21403	21%
ethyl acetate	293.15	0.185042	0.20687	0.16453	11%	0.24398	32%
toluene	293.15	0.169557	0.20687	0.18966	12%	0.14048	17%
methanol	303.15	0.213914	0.28268	0.20791	3%	0.20431	4%
ethanol	303.15	0.240779	0.28268	0.14555	40%	0.26258	9%
2-propanol	303.15	0.274236	0.28268	0.18170	34%	0.29569	8%
acetone	303.15	0.276451	0.28268	0.29650	7%	0.34288	24%
methyl isobutyl ketone	303.15	0.270510	0.28268	0.30148	11%	0.30165	12%
ethyl acetate	303.15	0.267821	0.28268	0.24842	7%	0.31959	19%
toluene	303.15	0.250865	0.28268	0.27058	8%	0.23333	7%
methanol	308.15	0.297768	0.32875	0.26377	11%	0.25186	15%
ethanol	308.15	0.332462	0.32875	0.19917	40%	0.31036	7%
2-propanol	308.15	0.309703	0.32875	0.23407	24%	0.34310	11%
acetone	308.15	0.320992	0.32875	0.34481	7%	0.38538	20%
methyl isobutyl ketone	308.15	0.316441	0.32875	0.34760	10%	0.34728	10%
ethyl acetate	308.15	0.316472	0.32875	0.30042	5%	0.36411	15%
toluene	308.15	0.299460	0.32875	0.31973	7%	0.28936	3%

Table F-14. Solubility of Monuron in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fina, Sharp et al. 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.00005489	0.018905			0.000061	11%
heptane	298.15	0.00005565	0.018905			0.000064	14%
octane	298.15	0.00006571	0.018905			0.000065	1%
nonane	298.15	0.00007811	0.018905			0.000067	14%
decane	298.15	0.00010076	0.018905			0.000068	32%
hexadecane	298.15	0.00008653	0.018905			0.000076	12%
cyclohexane	298.15	0.00005088	0.018905			0.000072	42%
methylcyclohexane	298.15	0.00007012	0.018905			0.000070	0%
2,2,4-trimethylpentane	298.15	0.00004697	0.018905			0.000049	5%
benzene	298.15	0.001365	0.018905			0.001365	0%
toluene	298.15	0.001155	0.018905			0.001030	11%
ethylbenzene	298.15	0.0007937	0.018905			0.000667	16%
dibutyl ether	298.15	0.001383	0.018905			0.001382	0%
tetrahydrofuran	298.15	0.02643	0.018905			0.026248	1%
1,2-dichloroethane	298.15	0.006743	0.018905			0.003798	44%
dichloromethane	298.15	0.009436	0.018905			0.007476	21%
chloroform	298.15	0.0124	0.018905			0.010734	13%
carbon tetrachloride	298.15	0.0003361	0.018905			0.000467	39%
butyl acetate	298.15	0.008675	0.018905			0.004825	44%
ethyl acetate	298.15	0.01007	0.018905			0.007395	27%
methanol	298.15	0.01264	0.018905			0.011104	12%
ethanol	298.15	0.01142	0.018905			0.010644	7%
1-propanol	298.15	0.01287	0.018905			0.010019	22%
2-propanol	298.15	0.008095	0.018905			0.008834	9%
1-butanol	298.15	0.01358	0.018905			0.010294	24%
2-butanol	298.15	0.009261	0.018905			0.008867	4%
2-methyl-1-propanol	298.15	0.0106	0.018905			0.008889	16%
2-methyl-2-propanol	298.15	0.006547	0.018905			0.012284	88%
1-pentanol	298.15	0.01483	0.018905			0.009501	36%
1-hexanol	298.15	0.01496	0.018905			0.008276	45%
1-octanol	298.15	0.01457	0.018905			0.007727	47%
1-decanol	298.15	0.0132	0.018905			0.006782	49%
cyclopentanol	298.15	0.01534	0.018905				
tert-butylcyclohexane	298.15	0.0000992	0.018905				
2-pentanol	298.15	0.01056	0.018905				
3-methyl-1-butanol	298.15	0.01249	0.018905				
2-methyl-2-butanol	298.15	0.004726	0.018905				
2-methyl-1-pentanol	298.15	0.01206	0.018905				
4-methyl-2-pentanol	298.15	0.008105	0.018905				
1-heptanol	298.15	0.01478	0.018905				
2-ethyl-1-hexanol	298.15	0.01096	0.018905				

Table F-15. Solubility of Naphthalene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Acree and Abraham 2001).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
Ethanol	298.15	0.0398	0.3058	0.0310	22%	0.0360	10%
1-Propanol	298.15	0.0505	0.3058	0.0466	8%	0.0535	6%
1-Butanol	298.15	0.0666	0.3058	0.0599	10%	0.0659	1%
1-Pentanol	298.15	0.0811	0.3058	0.0714	12%	0.0786	3%
n-Hexane	298.15	0.1168	0.3058	0.1047	10%	0.1167	0%
n-Heptane	298.15	0.1300	0.3058	0.1131	13%	0.1234	5%
n-Octane	298.15	0.1420	0.3058	0.1201	15%	0.1280	10%
n-Hexadecane	298.15	0.2043	0.3058	0.1592	22%	0.1621	21%
Cyclohexane	303.15	0.1825	0.3461	0.1706	6%	0.2213	21%
Methylcyclohexane	298.15	0.1470	0.3058	0.1409	4%	0.1546	5%
Benzene	298.15	0.2946	0.3058	0.3039	3%	0.3090	5%
Toluene	298.15	0.2920	0.3058	0.2999	3%	0.2949	1%
Ethylbenzene	298.15	0.2926	0.3058	0.2672	9%	0.2896	1%
Dichloromethane	298.15	0.3300	0.3058	0.2775	16%	0.3381	2%
Trichloromethane	298.15	0.3390	0.3058	0.3361	1%	0.3657	8%
Carbon tetrachloride	298.15	0.2591	0.3058	0.2545	2%	0.2836	9%
Trichloroethylene	296.15	0.3633	0.2907	0.2828	22%	0.3171	13%
Diiodomethane	301.85	0.2017	0.3352	0.2053	2%	0.1861	8%
1,1-Dichloroethane	298.15	0.3090	0.3058	0.2786	10%	0.3236	5%
1,2-Dichloroethane	298.15	0.3200	0.3058	0.3311	3%	0.3200	0%
Chlorobenzene	298.15	0.3110	0.3058	0.3187	2%	0.3015	3%
Methanol	298.15	0.0235	0.3058	0.0269	15%	0.0236	1%
2-Butanol	301.9	0.0656	0.3356	0.0694	6%	0.0739	13%
2-Methyl-1-propanol	309.5	0.0780	0.4028	0.0943	21%	0.0890	14%
2-Methyl-2-propanol	304.8	0.0652	0.3602	0.0569	13%	0.1008	55%
1-Hexanol	296.05	0.0860	0.2899	0.0751	13%	0.0685	20%
1-Octanol	298.55	0.1240	0.3088	0.1001	19%	0.0933	25%
Cyclohexanol	303	0.1580	0.3448	0.0996	37%	0.1567	1%
Acetone	297.4	0.2270	0.3000	0.2232	2%	0.1630	28%
Carbon disulfide	298.15	0.2830	0.3058	0.2940	4%	0.2959	5%
Nitrobenzene	298	0.2956	0.3046	0.2597	12%	0.2362	20%
Aniline	295.2	0.1540	0.2837	0.1607	4%	0.1367	11%
Pyridine	297.6	0.3032	0.3016	0.3133	3%	0.2083	31%
Perflouro-tripropylamine	298.15	0.0030					
trans-1,4-Dimethylcyclohexane	298.15	0.1500	0.3058	0.1977	32%		
1,2-Dibromoethane	298.15	0.3030	0.3058	0.2620	14%		
Methylcyclohexanol	303	0.1390					
Furfuryl alcohol	305.6	0.1094	0.3672				
Thiophene	303.2	0.3588	0.3465	0.3794	6%		

Table F-16. Solubility of p-Aminophenylacetic acid in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Gracin and Rasmuson 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
methanol	289.15	0.000784	0.000746			0.000212	73%
ethanol	289.15	0.000335	0.000746			0.000207	38%
2-propanol	289.15	0.000159	0.000746			0.000181	14%
acetone	289.15	0.002602	0.000746			0.001310	50%
methyl isobutyl ketone	289.15	0.000728	0.000746			0.000418	43%
chloroform	289.15	0.00071	0.000746			0.000628	12%
ethyl acetate	289.15	0.00035	0.000746			0.000596	70%
toluene	289.15	0.000731	0.000746			0.000094	87%
methanol	293.15	0.000911	0.000957			0.000277	70%
ethanol	293.15	0.000427	0.000957			0.000270	37%
2-propanol	293.15	0.000238	0.000957			0.000238	0%
acetone	293.15	0.00337	0.000957			0.001648	51%
methyl isobutyl ketone	293.15	0.001456	0.000957			0.000544	63%
ethyl acetate	293.15	0.000699	0.000957			0.000769	10%
methanol	298.15	0.000995	0.001295			0.000382	62%
ethanol	298.15	0.000548	0.001295			0.000374	32%
acetone	298.15	0.003561	0.001295			0.002179	39%
methyl isobutyl ketone	298.15	0.001667	0.001295			0.000751	55%
chloroform	298.15	0.001104	0.001295			0.001106	0%
ethyl acetate	298.15	0.001048	0.001295			0.001047	0%
toluene	298.15	0.000853	0.001295			0.000189	78%
ethanol	303.15	0.0007	0.001734			0.000514	27%
2-propanol	303.15	0.000397	0.001734			0.000459	16%
acetone	303.15	0.004818	0.001734			0.002856	41%
chloroform	303.15	0.001498	0.001734			0.001494	0%

Table F-17. Solubility of Phenanthrene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Acree and Abraham 2001).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
methanol	298.15	0.0059	0.2599	0.0098	67%	0.0046	21%
2-propanol	298.15	0.0098	0.2599	0.0163	67%	0.0101	4%
ethanol	298.15	0.0111	0.2599	0.0108	3%	0.0080	28%
2-butanol	298.15	0.0118	0.2599	0.0242	105%	0.0160	36%
1-propanol	298.15	0.0136	0.2599	0.0178	32%	0.0127	7%
1-butanol	298.15	0.0177	0.2599	0.0242	37%	0.0177	0%
2,2,4-trimethylpentane	298.15	0.0249	0.2599	0.0472	90%	0.0198	20%
1-pentanol	298.15	0.0249	0.2599	0.0298	20%	0.0217	13%
hexane	298.15	0.0319	0.2599	0.0375	18%	0.0342	7%
acetonitrile	298.15	0.0327	0.2599	0.1139	249%	0.0396	21%
cyclohexane	298.15	0.0365	0.2599	0.0612	68%	0.0835	129%
heptane	298.15	0.0389	0.2599	0.0427	10%	0.0376	3%
octane	298.15	0.0444	0.2599	0.0471	6%	0.0398	10%
methylcyclohexane	298.15	0.0457	0.2599	0.0630	38%	0.0580	27%
nonane	298.15	0.0479	0.2599	0.0508	6%	0.0425	11%
1-octanol	298.15	0.0542	0.2599	0.0435	20%	0.0252	54%
decane	298.15	0.0553	0.2599	0.0542	2%	0.0438	21%
hexadecane	298.15	0.0797	0.2599	0.0698	12%	0.0543	32%
dibutyl ether	298.15	0.0945	0.2599	0.1084	15%	0.0812	14%
aniline	298.15	0.1101	0.2599	0.1377	25%	0.0936	15%
carbon tetrachloride	298.15	0.1262	0.2599	0.1880	49%	0.1944	54%
ethyl acetate	298.15	0.1499	0.2599	0.1276	15%	0.1524	2%
tetrachloromethane	305.6	0.1768	0.3068	0.2364	34%	0.2460	39%
butyl acetate	298.15	0.1812	0.2599	0.1935	7%	0.1607	11%
tetrachloromethane	310	0.2084	0.3373	0.2695	29%	0.2805	35%
2-butanone	298.15	0.2090	0.2599	0.1830	12%	0.1710	18%
1,4-dioxane	298.15	0.2165	0.2599	0.2262	4%	0.2607	20%
benzene	305.2	0.2239	0.3042	0.3049	36%	0.2998	34%
toluene	299.8	0.2459	0.2698	0.2620	7%	0.2349	4%
pyridine	299.8	0.2459	0.2698	0.3082	25%	0.1651	33%
cyclohexanone	298.15	0.2716	0.2599	0.2178	20%	0.2116	22%
benzene	313.4	0.2836	0.3624	0.3643	28%	0.3601	27%
tetrahydrofuran	298.15	0.2884	0.2599	0.2416	16%	0.2407	17%
benzene	315	0.2990	0.3746	0.3767	26%	0.3727	25%
toluene	307.7	0.3011	0.3211	0.3145	4%	0.2888	4%
pyridine	307.7	0.3011	0.3211	0.3566	18%	0.2174	28%
2-methyl-1-propanol	298.15	0.0102	0.2599	0.0242	137%	0.0136	34%

Table F-18. Solubility of Phenylacetic acid in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Gracin and Rasmuson 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
water	293.15	0.00209	0.38769	0.00014	93%	0.00209	0%
methanol	293.15	0.40687	0.38769	0.33294	18%	0.38905	4%
ethanol	293.15	0.41121	0.38769	0.23520	43%	0.42561	4%
2-propanol	293.15	0.37889	0.38769	0.23262	39%	0.46386	22%
acetone	293.15	0.42321	0.38769	0.40902	3%	0.39837	6%
methyl isobutyl ketone	293.15	0.37151	0.38769	0.37573	1%	0.38886	5%
chloroform	293.15	0.35840	0.38769	0.45256	26%	0.26589	26%
ethyl acetate	293.15	0.34817	0.38769	0.31998	8%	0.38867	12%
toluene	293.15	0.20366	0.38769	0.27029	33%	0.26007	28%

Table F-19. Solubility of p-Hydroxybenzoic acid in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Gracin and Rasmuson 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
water	298.15	0.00080	0.02164	0.00121	52%	0.00080	0%
methanol	298.15	0.11421	0.02164	0.09990	13%	0.06769	41%
ethanol	298.15	0.12612	0.02164	0.04801	62%	0.08135	36%
2-propanol	298.15	0.13607	0.02164	0.03604	74%	0.08111	40%
1-octanol	298.15	0.11024	0.02164	0.01817	84%	0.10252	7%
acetone	298.15	0.11935	0.02164	0.15278	28%	0.13152	10%
methyl isobutyl ketone	298.15	0.10011	0.02164	0.09087	9%	0.06109	39%
ethyl acetate	298.15	0.06984	0.02164	0.06288	10%	0.07723	11%
toluene	298.15	0.00100	0.02164	0.00076	24%	0.00100	0%

Table F-20. Solubility of p-Hydroxyphenylacetic acid in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Gracin and Rasmuson 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
water	283.15	0.003493	0.03616	0.00066	81%	0.00017	95%
methanol	283.15	0.164416	0.03616	0.13924	15%	0.04970	70%
ethanol	283.15	0.146704	0.03616	0.08159	44%	0.06388	56%
2-propanol	283.15	0.110495	0.03616	0.06413	42%	0.06802	38%
acetone	283.15	0.153599	0.03616	0.21310	39%	0.27085	76%
methyl isobutyl ketone	283.15	0.089216	0.03616	0.15370	72%	0.06184	31%
chloroform	283.15	0.001019	0.03616			0.00124	22%
ethyl acetate	283.15	0.072108	0.03616	0.11293	57%	0.10471	45%
toluene	283.15	0.001028	0.03616	0.00142	38%	0.00104	1%
water	288.15	0.004374	0.04196	0.00077	82%	0.00018	96%
methanol	288.15	0.182624	0.04196	0.15047	18%	0.05735	69%
ethanol	288.15	0.175361	0.04196	0.09386	46%	0.07316	58%
2-propanol	288.15	0.136112	0.04196	0.07477	45%	0.07800	43%
acetone	288.15	0.188522	0.04196	0.22210	18%	0.27603	46%
methyl isobutyl ketone	288.15	0.095938	0.04196	0.16188	69%	0.06956	27%
chloroform	288.15	0.001958	0.04196			0.00169	14%
ethyl acetate	288.15	0.078791	0.04196	0.12312	56%	0.11397	45%
toluene	288.15	0.001252	0.04196	0.00178	42%	0.00141	12%
water	293.15	0.005453	0.04855	0.00090	84%	0.00021	96%
methanol	293.15	0.252959	0.04855	0.16208	36%	0.06587	74%
ethanol	293.15	0.221104	0.04855	0.10739	51%	0.08335	62%
2-propanol	293.15	0.163899	0.04855	0.08676	47%	0.08894	46%
acetone	293.15	0.209197	0.04855	0.23157	11%	0.28201	35%
methyl isobutyl ketone	293.15	0.105783	0.04855	0.17061	61%	0.07811	26%
ethyl acetate	293.15	0.090494	0.04855	0.13410	48%	0.12399	37%
water	298.15	0.007136	0.05601	0.00105	85%	0.00026	96%
methanol	298.15	0.358862	0.05601	0.17409	51%	0.07532	79%
ethanol	298.15	0.307429	0.05601	0.12216	60%	0.09447	69%
2-propanol	298.15	0.191945	0.05601	0.10010	48%	0.10087	47%
acetone	298.15	0.221303	0.05601	0.24156	9%	0.28879	30%
methyl isobutyl ketone	298.15	0.116497	0.05601	0.17995	54%	0.08755	25%
ethyl acetate	298.15	0.100061	0.05601	0.14592	46%	0.13481	35%

Table F-21. Solubility of p-Nitroaniline in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Huyskens, Morissen et al. 1998).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
Nitromethane	298	0.042189	0.09753			0.02302	45%
Nitroethane	298	0.049872	0.09753			0.03814	24%
1-Nitropropane	298	0.039477	0.09753			0.05344	35%
2-Nitropropane	298	0.040539	0.09753			0.01983	51%
Acetonitrile	298	0.066945	0.09753			0.06204	7%
Propionitrile	298	0.080092	0.09753			0.07015	12%
Butyronitrile	298	0.085752	0.09753			0.11136	30%
Valeronitrile	298	0.08087	0.09753			0.10767	33%
Diethyl Ether	298	0.014941	0.09753			0.00914	39%
methyl tert-butyl ether	298	0.027712	0.09753			0.01856	33%
propyl ether	298	0.005801	0.09753			0.00405	30%
butyl ether	298	0.003341	0.09753			0.00338	1%
1,4-dioxane	298	0.156641	0.09753			0.10563	33%
tetrahydrofuran	298	0.174706	0.09753			0.20716	19%
acetone	298	0.156872	0.09753	0.07139	54%	0.16640	6%
2-butanone	298	0.152369	0.09753	0.05647	63%	0.15022	1%
isobutyl methyl ketone	298	0.114112	0.09753	0.03849	66%	0.03217	72%
2-pentanone	298	0.139897	0.09753	0.04602	67%	0.07946	43%
methyl acetate	298	0.13257	0.09753			0.06584	50%
ethyl acetate	298	0.09025	0.09753			0.05067	44%
n-propyl acetate	298	0.080344	0.09753			0.04228	47%
n-butyl acetate	298	0.068058	0.09753	0.03849	43%	0.02609	62%
n-pentyl acetate	298	0.06248	0.09753	0.03291	47%	0.01375	78%
DMSO	298	0.324413	0.09753			0.57410	77%
Chloroform	298	0.008672	0.09753			0.00992	14%
Dichloromethane	298	0.01344	0.09753			0.02145	60%
1,2-dichloroethane	298	0.016776	0.09753			0.01780	6%
1-chlorobutane	298	0.002502	0.09753	0.00629	151%	0.00121	52%
methanol	298	0.017034	0.09753			0.02092	23%
ethanol	298	0.020046	0.09753	0.00454	77%	0.01716	14%
1-propanol	298	0.015462	0.09753	0.00452	71%	0.01088	30%
1-butanol	298	0.014413	0.09753	0.00444	69%	0.01440	0%
isobutanol	298	0.008732	0.09753	0.00444	49%	0.01073	23%
1-pentanol	298	0.012511	0.09753	0.00437	65%	0.01159	7%
1-hexanol	298	0.014213	0.09753	0.00431	70%	0.00924	35%
1-octanol	298	0.01071	0.09753	0.00424	60%	0.01098	3%
2-propanol	298	0.015291	0.09753	0.00390	75%	0.01136	26%
2-butanol	298	0.012918	0.09753	0.00444	66%	0.01033	20%
tert-butanol	298	0.016838	0.09753	0.00245	85%	0.02290	36%
5-nonanone	298	0.088745	0.09753	0.01742	80%	0.01070	
4-heptanone	298	0.101591	0.09753	0.02363			
tetrahydropyran	298	0.120575	0.09753				

Table F-22. Solubility of N,N-dimethyl-p-nitroaniline in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Huyskens, Morissen et al. 1998).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
Nitromethane	298.15	0.01670	0.02684			0.00905	46%
Nitroethane	298.15	0.01815	0.02684			0.01607	12%
1-Nitropropane	298.15	0.01965	0.02684			0.01829	7%
2-Nitropropane	298.15	0.01581	0.02684			0.01545	2%
Acetonitrile	298.15	0.00774	0.02684			0.00852	10%
Propionitrile	298.15	0.01174	0.02684			0.01686	44%
Butyronitrile	298.15	0.01526	0.02684			0.01746	14%
Valeronitrile	298.15	0.01696	0.02684				
1,4-dioxane	298.15	0.01074	0.02684			0.02589	141%
tetrahydrofuran	298.15	0.02064	0.02684			0.01349	35%
tetrahydropyran	298.15	0.01176	0.02684				
acetone	298.15	0.01419	0.02684			0.01141	20%
2-butanone	298.15	0.01743	0.02684			0.01493	14%
2-pentanone	298.15	0.01792	0.02684			0.01337	25%
4-heptanone	298.15	0.01548	0.02684				
5-nonanone	298.15	0.01366	0.02684			0.01060	22%
methyl acetate	298.15	0.00981	0.02684			0.01018	4%
ethyl acetate	298.15	0.00942	0.02684			0.01171	24%
n-propyl acetate	298.15	0.00919	0.02684			0.00849	8%
n-butyl acetate	298.15	0.00862	0.02684			0.00926	7%
n-pentyl acetate	298.15	0.00862	0.02684				
DMSO	298.15	0.01541	0.02684			0.01540	0%
Chloroform	298.15	0.04204	0.02684			0.04109	2%
Dichloromethane	298.15	0.03703	0.02684			0.03880	5%
1,2-dichloroethane	298.15	0.02874	0.02684			0.03270	14%
1-chlorobutane	298.15	0.00620	0.02684			0.00761	23%
methanol	298.15	0.00094	0.02684			0.00083	11%
ethanol	298.15	0.00120	0.02684			0.00093	22%
1-propanol	298.15	0.00126	0.02684			0.00104	17%
1-butanol	298.15	0.00136	0.02684			0.00133	2%
isobutanol	298.15	0.00098	0.02684			0.00108	10%
1-pentanol	298.15	0.00139	0.02684			0.00141	1%
1-hexanol	298.15	0.00161	0.02684			0.00120	25%
1-octanol	298.15	0.00156	0.02684			0.00132	15%
2-propanol	298.15	0.00088	0.02684			0.00090	2%
2-butanol	298.15	0.00104	0.02684			0.00111	7%
tert-butanol	298.15	0.00093	0.02684			0.00175	89%

Table F-23. Solubility of Pyrene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Hansen, Riverol et al. 2000).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	299.15	0.00852	0.12833	0.00791	7%	0.00754	12%
heptane	299.15	0.01101	0.12833	0.00952	14%	0.00852	23%
octane	299.15	0.01379	0.12833	0.01094	21%	0.00918	33%
cyclohexane	299.15	0.01089	0.12833	0.01472	35%	0.01918	76%
methylcyclohexane	299.15	0.01300	0.12833	0.01546	19%	0.01345	3%
2,2,4-trimethylpentane	299.15	0.00721	0.12833	0.01099	52%	0.00421	42%
cyclooctane	299.15	0.01956	0.12833	0.01380	29%	0.01957	0%
benzene	299.15	0.06316	0.12833	0.10973	74%	0.12015	90%
toluene	299.15	0.06785	0.12833	0.10611	56%	0.09465	40%
p-xylene	299.15	0.06831	0.12833	0.10114	48%	0.06509	5%
methanol	299.15	0.00149	0.12833	0.00287	92%	0.00153	3%
ethanol	299.15	0.00317	0.12833	0.00333	5%	0.00247	22%
1-propanol	299.15	0.00426	0.12833	0.00544	28%	0.00387	9%
2-propanol	299.15	0.00290	0.12833	0.00456	57%	0.00290	0%
1-butanol	299.15	0.00622	0.12833	0.00735	18%	0.00535	14%
2-butanol	299.15	0.00433	0.12833	0.00735	70%	0.00463	7%
2-methyl-1-propanol	299.15	0.00319	0.12833	0.00735	130%	0.00394	23%
1-pentanol	299.15	0.00926	0.12833	0.00905	2%	0.00659	29%
1-octanol	299.15	0.02097	0.12833	0.01325	37%	0.00706	66%
acetone	299.15	0.03612	0.12833	0.04958	37%	0.03606	0%
dibutyl ether	299.15	0.02980	0.12833	0.02845	5%	0.02241	25%
dioxane	299.15	0.03520	0.12833	0.07436	111%	0.13409	281%
ethyl acetate	299.15	0.04251	0.12833	0.02543	40%	0.05465	29%
butyl acetate	299.15	0.05932	0.12833	0.06433	8%	0.05788	2%
carbon tetrachloride	299.15	0.04229	0.12833	0.05383	27%	0.06803	61%
1,2-dichloroethane	299.15	0.08746	0.12833	0.10202	17%	0.14454	65%
1-chlorobutane	299.15	0.06094	0.12833	0.02894	53%	0.06478	6%
1,4-dichlorobutane	299.15	0.10970	0.12833	0.05807	47%		
tert-butylcyclohexane	299.15	0.01590	0.12833	0.01821	15%		
m-xylene	299.15	0.07055	0.12833	0.10114	43%		

Table F-24. Solubility of Thianthrene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Fletcher, McHale et al. 1997).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.0032	0.04435			0.00320	0%
heptane	298.15	0.00346	0.04435			0.00374	8%
octane	298.15	0.00392	0.04435			0.00415	6%
cyclohexane	298.15	0.00587	0.04435			0.00807	37%
methylcyclohexane	298.15	0.00631	0.04435			0.00585	7%
cyclooctane	298.15	0.01232	0.04435			0.00937	24%
2,2,4-trimethylpentane	298.15	0.00273	0.04435			0.00187	32%
dibutyl ether	298.15	0.0097	0.04435			0.00763	21%
methanol	298.15	0.000472	0.04435			0.00061	29%
ethanol	298.15	0.001038	0.04435			0.00095	8%
1-propanol	298.15	0.00162	0.04435			0.00162	0%
2-propanol	298.15	0.001007	0.04435			0.00109	8%
1-butanol	298.15	0.00227	0.04435			0.00207	9%
2-butanol	298.15	0.00166	0.04435			0.00180	8%
2-methyl-1-propanol	298.15	0.00149	0.04435			0.00149	0%
1-pentanol	298.15	0.00308	0.04435			0.00272	12%
1-hexanol	298.15	0.0039	0.04435			0.00234	40%
1-heptanol	298.15	0.00501	0.04435				
1-octanol	298.15	0.00553	0.04435			0.00299	46%
tert-butylcyclohexane	298.15	0.00658	0.04435				

Table F-25. Solubility of trans-Stilbene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Abraham, Green et al. 1998).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.009516	0.07525	0.01387	46%	0.01059	11%
heptane	298.15	0.010899	0.07525	0.01553	42%	0.01163	7%
octane	298.15	0.012393	0.07525	0.01690	36%	0.01230	1%
nonane	298.15	0.013938	0.07525	0.01809	30%	0.01309	6%
decane	298.15	0.015201	0.07525	0.01915	26%	0.01349	11%
hexadecane	298.15	0.02181	0.07525	0.02418	11%	0.01661	24%
2,2,4-trimethylpentane	298.15	0.00792	0.07525	0.01695	114%	0.00635	20%
cyclohexane	298.15	0.013704	0.07525	0.01783	30%	0.02211	61%
carbon tetrachloride	298.15	0.038672	0.07525	0.05655	46%	0.06421	66%
acetonitrile	298.15	0.009619	0.07525	0.02217	130%	0.00962	0%
benzene	298.15	0.059116	0.07525	0.08424	42%	0.08666	47%
toluene	298.15	0.05861	0.07525	0.07954	36%	0.07262	24%
chlorobenzene	298.15	0.070767	0.07525	0.09950	41%	0.07866	11%
methanol	298.15	0.001942	0.07525	0.00234	20%	0.00194	0%
ethanol	298.15	0.003148	0.07525	0.00269	15%	0.00313	1%
1-octanol	298.15	0.012569	0.07525	0.01263	0%	0.00890	29%

Table F-26. Solubility of Xanthrene in various solvents with predictions by UNIFAC and MOSCED. Experimental data (Monárrez, Stovall et al. 2002).

Solvent	T	x^{exp}	x^{id}	UNIFAC	Error	MOSCED	Error
hexane	298.15	0.02949	0.2091	0.0420	43%	0.0297	1%
heptane	298.15	0.03543	0.2091	0.0452	27%	0.0336	5%
octane	298.15	0.03976	0.2091	0.0476	20%	0.0364	8%
nonane	298.15	0.04306	0.2091	0.0495	15%	0.0396	8%
decane	298.15	0.0461	0.2091	0.0513	11%	0.0414	10%
hexadecane	298.15	0.06835	0.2091	0.0596	13%	0.0546	20%
cyclohexane	298.15	0.04203	0.2091	0.0524	25%	0.0697	66%
methylcyclohexane	298.15	0.04275	0.2091	0.0549	28%	0.0507	19%
cyclooctane	298.15	0.05414	0.2091	0.0445	18%	0.0738	36%
2,2,4-trimethylpentane	298.15	0.02451	0.2091	0.0477	95%	0.0180	27%
dibutyl ether	298.15	0.0831	0.2091	0.1199	44%	0.0624	25%
methyl tert-butyl ether	298.15	0.07846	0.2091	0.1501	91%	0.0844	8%
1,2-dichloroethane	298.15	0.1546	0.2091	0.3100	101%	0.1864	21%
carbon tetrachloride	298.15	0.1237	0.2091	0.2439	97%	0.1389	12%
acetonitrile	298.15	0.0197	0.2091	0.0886	350%	0.0197	0%
methanol	298.15	0.004455	0.2091	0.0119	168%	0.0036	19%
ethanol	298.15	0.006231	0.2091	0.0111	79%	0.0063	1%
1-propanol	298.15	0.01166	0.2091	0.0184	58%	0.0105	10%
2-propanol	298.15	0.008643	0.2091	0.0191	121%	0.0080	8%
1-butanol	298.15	0.01756	0.2091	0.0248	41%	0.0142	19%
2-butanol	298.15	0.01254	0.2091	0.0248	98%	0.0129	3%
2-methyl-1-propanol	298.15	0.01077	0.2091	0.0248	131%	0.0108	0%
2-methyl-2-propanol	298.15	0.01112	0.2091	0.0189	70%	0.0176	58%
1-pentanol	298.15	0.02212	0.2091	0.0305	38%	0.0182	18%
1-hexanol	298.15	0.02831	0.2091	0.0354	25%	0.0162	43%
1-octanol	298.15	0.038	0.2091	0.0438	15%	0.0217	43%
1-decanol	298.15	0.04528	0.2091	0.0507	12%	0.0528	17%
cyclopentanol	298.15	0.02886	0.2091	0.0280	3%		
2-pentanol	298.15	0.01766	0.2091	0.0215	22%		
3-methyl-1-butanol	298.15	0.01633	0.2091	0.0241	48%		
2-methyl-2-butanol	298.15	0.01946	0.2091	0.0305	57%		
2-methyl-1-pentanol	298.15	0.01969	0.2091	0.0354	80%		
4-methyl-2-pentanol	298.15	0.01762	0.2091	0.0355	102%		
1-heptanol	298.15	0.0334	0.2091	0.0354	6%		

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APPENDIX G

EXPERIMENTAL SOLID SOLUBILITY DATA IN PURE AND MIXED SOLVENTS

Table G-1. Solubility of 2-amino-5-nitrobenzophenone in various solvents at 286 K, 298 K, and 308 K.

Solvent	286 K	298 K	308 K
cyclohexane	--	0.00073	--
toluene	0.00208	0.00206	0.00352
methanol	--	0.00166	--
ethanol	0.00063	0.00118	0.00189
2-propanol	0.00056	0.00097	0.00199
benzyl alcohol	--	0.01699	--
ethyl acetate	0.02232	0.03074	0.04741
2-butanone	0.03437	0.05064	0.08275
nitromethane	0.01008	0.01905	0.02234
dioxane	0.02794	0.04215	0.05660
acetonitrile	0.00641	0.01082	0.01885
benzonitrile	--	0.05294	--
chloroform	0.02022	0.03005	0.03200
dichloromethane	0.02416	0.03804	0.04260
chlorobenzene	--	0.00594	--

Table G-2. Solubility of 2-amino-5-nitrobenzophenone in mixed solvents (solute free mole ratio) of ethyl acetate (EtAc), Ethanol (EtOH), and Nitromethane (Nitro) at 298 K.

T (K)	Solvent	x^{exp}
298	1 EtAc/ 0 EtOH	0.03074
298	0.75 EtAc/ 0.25 EtOH	0.00990
298	0.50 EtAc/ 0.50 EtOH	0.00799
298	0.25 EtAc /0.75 EtOH	0.00379
298	0 EtAc/ 1 EtOH	0.00118
298	1 Nitro/ 0 EtOH	0.01996
298	0.75 Nitro/ 0.25 EtOH	0.00539
298	0.50 Nitro/ 0.50 EtOH	0.00249
298	0.25 Nitro /0.75 EtOH	0.00263
298	0 Nitro/ 1 EtOH	0.00121

Table G-3. Solubility of 5-fluoroisatin in various solvents at 286 K, 298 K, and 308 K.

Solvent	286 K	298 K	308 K
cyclohexane	--	0.00054	--
toluene	0.00183	0.00082	0.00132
ethanol	0.00412	0.00543	0.00533
2-propanol	0.00358	0.00474	0.00642
ethyl acetate	0.00924	0.01067	0.01667
2-butanone	0.00971	0.01422	0.02775
nitromethane	0.00589	0.00629	0.00826
dioxane	0.01639	0.02055	0.03484
acetonitrile	0.00658	0.00815	0.01018
N,N-dimethylformamide	--	0.07713	--
N-methyl-2-pyrrolidone	--	0.13526	--
chloroform	0.00149	0.00336	0.00224
dichloromethane	0.00082	0.00115	0.00178

Table G-4. Solubility of 5-fluoroisatin in mixed solvents (solute free mole ratio) of ethyl acetate (EtAc), Ethanol (EtOH), and Nitromethane (Nitro) at 298 K.

T (K)	Solvent	x^{exp}
298	1 EtAc/ 0 EtOH	0.01067
298	0.75 EtAc/ 0.25 EtOH	0.01396
298	0.50 EtAc/ 0.50 EtOH	0.01903
298	0.25 EtAc /0.75 EtOH	0.01267
298	0 EtAc/ 1 EtOH	0.00543
298	1 Nitro/ 0 EtOH	0.00629
298	0.75 Nitro/ 0.25 EtOH	0.01168
298	0.50 Nitro/ 0.50 EtOH	0.01593
298	0.25 Nitro /0.75 EtOH	0.01272
298	0 Nitro/ 1 EtOH	0.00543

Table G-5. Solubility of 3-nitrophthalimide in various solvents at 286 K, 298 K, and 308 K.

Solvent	286 K	298 K	308 K
cyclohexane	0.00005	0.00014	0.00021
toluene	0.00014	0.00025	0.00041
ethanol	0.00073	0.00125	0.00291
2-propanol	0.00046	0.00061	0.00126
ethyl acetate	0.00480	0.00741	0.00994
2-butanone	0.00893	0.01253	0.01704
nitromethane	0.00320	0.00541	0.00787
dioxane	--	0.01020	0.01799
acetonitrile	0.00406	0.00640	0.00904
DMF	--	0.20732	--
NMP	--	0.39590	--
chloroform	--	0.00052	--
dichloromethane	0.00037	0.00073	0.00164

Table G-6. Solubility of 3-nitrophthalimide in mixed solvents (solute free mole ratio) of ethyl acetate (EtAc), Ethanol (EtOH), and Nitromethane (Nitro) at 298 K.

T (K)	Solvent	x^{exp}
298	1 EtAc/ 0 EtOH	0.0076
298	0.75 EtAc/ 0.25 EtOH	0.0080
298	0.50 EtAc/ 0.50 EtOH	0.0073
298	0.25 EtAc /0.75 EtOH	0.0036
298	0 EtAc/ 1 EtOH	0.0013
298	1 Nitro/ 0 EtOH	0.0058
298	0.75 Nitro/ 0.25 EtOH	0.0110
298	0.50 Nitro/ 0.50 EtOH	0.0082
298	0.25 Nitro /0.75 EtOH	0.0046
298	0 Nitro/ 1 EtOH	0.0013

Table G-7. Solubility of 2-aminopyrimidine in various solvents at 298 K.

T (K)	Solvent	x^{exp}
298	methanol	0.0669
298	2-propanol	0.0363
298	ethyl acetate	0.0477
298	2-butanone	0.0510
298	nitromethane	0.0343
298	dioxane	0.0572
298	acetonitrile	0.0320
298	N,N-dimethylformamide	0.2033
298	chloroform	0.0708
298	dichloromethane	0.0453

Table G-8. Solubility of 2-aminopyrimidine in mixed solvents (solute free mole ratio) of ethyl acetate (EtAc), Methanol (MeOH), and Nitromethane (Nitro), Acetonitrile (AcN), and 1,4-Dioxane (Diox) at 298 K.

T (K)	Solvent	x^{exp}
298	1 EtAc/ 0 MeOH	0.048
298	0.75 EtAc/ 0.25 MeOH	0.081
298	0.50 EtAc/ 0.50 MeOH	0.098
298	0.25 EtAc /0.75 MeOH	0.092
298	0 EtAc/ 1 MeOH	0.067
298	1 Nitro/ 0 MeOH	0.034
298	0.75 Nitro/ 0.25 MeOH	0.085
298	0.50 Nitro/ 0.50 MeOH	0.110
298	0.25 Nitro /0.75 MeOH	0.110
298	0 Nitro/ 1 MeOH	0.067
298	1 AcN/ 0 MeOH	0.032
298	0.75 AcN/ 0.25 MeOH	0.058
298	0.50 AcN/ 0.50 MeOH	0.080
298	0.25 AcN /0.75 MeOH	0.086
298	0 AcN/ 1 MeOH	0.067
298	1 AcN/ 0 Diox	0.032
298	0.75 AcN/ 0.25 Diox	0.041
298	0.50 AcN/ 0.50 Diox	0.054
298	0.25 AcN /0.75 Diox	0.078
298	0 AcN/ 1 Diox	0.057

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VITA

Michael John Lazzaroni was born in Tampa, Florida on July 30, 1977. He was lovingly reared by his parents, Michael E. and Mary Kay Lazzaroni, in nearby Riverview. He attended high school at East Bay Sr. High in Gibsonton, FL. Michael graduated *cum laude* from the University of South Florida in December, 1999 with a Bachelor of Science in Chemical Engineering and continued studies in trumpet performance. While at USF, he met his beautiful wife, Kimberly, whom he married in May, 2004. In 2000 he was admitted to the Georgia Institute of Technology. His graduate studies were directed by Professor Charles A. Eckert and Professor Charles L. Liotta. He will complete his Ph.D. in Chemical Engineering in the summer of 2004. Selected publications and presentations are listed above.