

The Measurement of Flash Point for Binary Mixtures of 2,2,4-Trimethylpentane, Methylcyclohexane, Ethylbenzene and *p*-xylene at 101.3 kPa

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Abstract

Laboratories and industrial processes typically involve the use of flammable substances. An important property used to estimate fire and explosion risk for a flammable liquid is the flash point. In this study, flash point data at 101.3 kPa were determined using a SETA closed cup flash point tester on the following solvent mixtures: {2,2,4-trimethylpentane + methylcyclohexane}, {2,2,4-trimethylpentane + ethylbenzene}, and {2,2,4-trimethylpentane + *p*-xylene}. The purpose of this work is to obtain flash point data for binary mixtures of 2,2,4-trimethylpentane with three hydrocarbons (methylcyclohexane, ethylbenzene, and *p*-xylene), which are representative compounds of the main aromatic hydrocarbon fractions of petroleum. The measured flash points are compared with the predicted values calculated using the G^E models' activity coefficient patterns: the Wilson, the Non-Random Two-Liquid (NRTL), and the UNiversal QUAsiChemical (UNIQUAC) models. The non-ideality of the mixture is also considered. The average absolute deviation between the predicted and measured lower flash points is less than 1.99 K, except when Raoult's law is calculated. In addition, the minimum flash point behavior is not observed in any of the three binary systems. This work's predicted results can be applied to design safe petrochemical processes, such as identifying safe storage conditions for non-ideal solutions containing volatile components.

Keywords : Flash point, Seta closed cup tester, Binary system, G^E models

1. Introduction

For the design of prevention and mitigation measures in process industries involving flammable substances, reliable safety data are required. An important property used to estimate the risk of fire and explosion for a flammable liquid is the flash point (*FP*) [1,2]. Flammability is an important factor to consider when developing safe methods for storing and handling solids and liquids [3]. For a given liquid, the *FP* is the temperature determined experimentally at which the substance emits sufficient vapor to form a combustible mixture with air. Flammable substances are commonly used in laboratories and industry; thus, it is important to consider the physical properties of the substances to avoid any associated hazards. The lower flammable limit (*LFL*) provides information on the fundamental physical processes of combustion. Experimental *FP* data have become important in ensuring safe storage of flammable

substances and, for this reason, studies for predicting the *FP* of pure substances and mixtures are increasingly important. Recently, several methods have been developed for the prediction or estimation of low *FP* of pure compound and mixtures [4-6].

Methylcyclohexane, ethylbenzene, *p*-xylene, and their mixtures are frequently used in the tire, rubber, and polymer manufacturing industries [7-9], whereas 2,2,4-trimethylpentane is used as a solvent in the manufacture of chemicals, adhesives, and coatings, and as an ingredient in aviation fuel and gasoline [10]. It is also used as a fuel additive, non-polar solvent, and volatile organic compound. The separation of these compounds is one of the most dangerous processes in the petrochemical industry. To simulate and optimize the separation process, it is essential to describe *FP* data accurately. The purpose of this work was to obtain *FP* data for binary mixtures of 2,2,4-trimethylpentane with the three hydrocarbons (methylcyclohexane, ethylbenzene, and *p*-xylene), which are representative compounds of the main aromatic

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Table 1. The purities, *FPs* and UNIQUAC parameters of chemicals used in this work.

Chemicals	G.C. analysis (wt %)	Flash Point (K) at 101.3 kPa		UNIQUAC	
		This work	Reference ^a	r-value ^b	q-value ^b
2,2,4-trimethylpentane	> 99.8	265.45	268.65	5.8462	4.9240
Methylcyclohexane	> 99.8	268.45	269.15	4.7200	3.7760
Ethylbenzene	> 99.7	295.35	294.15	4.5972	3.5080
<i>p</i> -xylene	> 99.9	299.45	300.15	4.6578	3.5360

^a Ref. [14], ^b Ref. [15]

hydrocarbon fractions of petroleum.

In the present work, the *FPs* at 101.3 kPa were determined using a SETA closed cup flash point tester on the following solvent mixtures: {2,2,4-trimethylpentane (1) + methylcyclohexane (2)}, {2,2,4-trimethylpentane (1) + ethylbenzene (2)} and {2,2,4-trimethylpentane (1) + *p*-xylene (2)}. The experimental *FP* data for these binary systems were compared with predicted values from a variety of activity coefficient models: Wilson, Non-Random Two-Liquid (NRTL) and UNIversal QUAsiChemical (UNIQUAC) models [11-13].

2. Material and Methods

2.1. Materials

Commercial grade 2,2,4-trimethylpentane (C₈H₁₈, *M* = 114.23 g mol⁻¹, CAS-RN 540-84-1, 99.8%) and methylcyclohexane (C₇H₁₄, *M* = 98.19 g mol⁻¹, CAS-RN 108-87-2, 99.8%) were supplied from Aldrich Chemical Co. Ethylbenzene (C₈H₁₀, *M* = 106.17 g mol⁻¹, CAS-RN 100-41-4, 99.5%) and *p*-xylene (C₈H₁₀, *M* = 106.17 g mol⁻¹, CAS-RN 106-42-3, 99.9%) were supplied from Fluka Co. All components were dried using molecular sieves of pore diameter 0.4 nm. The water content of the chemicals, determined using a Karl-Fischer titrator (Metrohm 684 KF-Coulometer), was less than 6 × 10⁻⁵ g g⁻¹. The purity of the chemicals was assessed through gas chromatography. The purities, *FPs*, and UNIQUAC parameters of the chemicals are listed in Table 1 along with the reported values [14,15].

2.2. Procedure

SETA closed-cup flash point tester (Series 8 SETAFLASH, model 82000-0, Surrey, UK) was used to measure the *FPs* of the three miscible mixtures. The SETA closed-cup flash point tester was operated according to the standard test method, ASTM D 3278 [16]. The abovementioned tester comprises four components: a sample cup, a test flame device with a flame controller, a temperature-measuring system with a temperature controller, and a time controller. The injection volume was 2 mL, and the measured temperature range was set from 253.15

to 573.15 K. The temperature of the liquid sample in the sample cup was regulated using the temperature controller, which had an accuracy of ± 0.1 K. The SETA closed-cup flash point tester was calibrated periodically using a standard tester solvent. Approximately 2 mL of the sample mixture was weighed using a microbalance (Ohaus DV215CD) of precision 1 × 10⁻⁵ g. The heavier component of the binary mixtures was weighed first to minimize vaporization. The systematic error associated with the experiments was estimated to be less than 1 × 10⁻⁴ in terms of molefraction. A time interval of 15 min was imposed between measurements to attain a constant temperature and stabilize oscillations. The experimental procedure is described in detail elsewhere [17-19].

3. Results and Discussion

At the *FP* of a liquid solution, the *Le Chatelier's* principle [20], which describes the lower flammable limit of a gas mixture, is expressed as follows:

$$1 = \sum_i \frac{y_i}{LFL_i} \quad (1)$$

where y_i is the vapor phase composition of a flammable substance i and LFL_i is the lower flammable limit of the pure component i . LFL_i is expressed in terms of the vapor pressure of i at its *FP*, i.e., $P_{i,FP}^{sat}$, as follows:

$$LFL_i = \frac{P_{i,FP}^{sat}}{P} \quad (2)$$

where P represents the ambient pressure. The *FP* of a pure substance is typically measured at the standard atmospheric pressure. Under this condition, the vapor phase behaves ideally. In a liquid mixture containing flammable substances in the presence of non-condensable components of air, the vapor-liquid equilibrium of component i is described by the following equation:

$$y_i P = x_i \gamma_i P_i^{sat} \quad (3)$$

Table 2. The Antoine coefficients of the components

Components	Antoine coefficients ^a		
	A	B	C
2,2,4-trimethylpentane	6.96602	1339.49	229.033
Methylcyclohexane	6.83900	1278.57	222.168
Ethylbenzene	6.96580	1429.55	213.767
<i>p</i> -xylene	6.99053	1453.43	215.300

^a Ref. [15]

In Equation (3), γ_i , x_i , and y_i are the liquid phase activity coefficient, liquid molar fraction, and vapor molar fraction, respectively.

As proposed by Liaw et al. [21], one can substitute Equations (2) and (3) into Equation (1), resulting in Equation (4), which allows the evaluation of *FPs* for flammable liquid mixtures.

$$\sum_i \frac{x_i \gamma_i P_i^{sat}}{P_{i,FP}^{sat}} = 1 \quad (4)$$

The saturated vapor pressure variation with temperature for a pure substance *i* can be obtained using the Antoine equation as follows [22]:

$$\log P^{sat} (mmHg) = A - \frac{B}{C + T/^\circ C} \quad (5)$$

The Antoine coefficients A, B, and C were adapted from the literature and are listed in Table 2.

According to being proposed by Liaw et al. [21], the substitution Equation (2) and Equation (3) into Equation (1) results in:

$$\sum_i \frac{x_i \gamma_i P_i^{sat}}{P_{i,FP}^{sat}} = \frac{x_1 \gamma_1 P_1^{sat}}{P_{1,FP}^{sat}} + \frac{x_2 \gamma_2 P_2^{sat}}{P_{2,FP}^{sat}} = 1 \quad (6)$$

$P_{i,FP}^{sat}$, presented in Equation (6), can be calculated by substituting the *FP* of the pure component *i* into Equation (5). Assuming that the solution is ideal, the activity coefficients of the liquid phase are equal to unity. Therefore, Equation (4) was reduced according to Raoult's law and is expressed as follows [23]:

$$\sum_i \frac{x_i P_i^{sat}}{P_{i,FP}^{sat}} = \frac{x_1 P_1^{sat}}{P_{1,FP}^{sat}} + \frac{x_2 P_2^{sat}}{P_{2,FP}^{sat}} = 1 \quad (7)$$

The temperature that satisfies Equation (7) is determined to be the *FP* of the binary mixture. For non-ideal liquid mixtures, the activity coefficients (γ_i) were estimated using the optimum binary interaction parameters of the Wilson, NRTL, and UNIQUAC equations, described below [11-13].

Wilson equation:

$$\ln \gamma_i = -\ln\left(\sum_{j=1}^n x_j \Lambda_{ij}\right) + 1 - \sum_{k=1}^n \frac{x_j \Lambda_{ji}}{\sum_{j=1}^n x_j \Lambda_{kj}} \quad (8)$$

with

$$\Lambda_{ij} = \frac{V_j^2}{V_i^2} \exp\left(-\frac{\lambda_{ij} - \lambda_{ii}}{RT}\right)$$

NRTL equation:

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ij}}{\sum_k G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k x_k \tau_{kj} G_{kj}}{\sum_k G_{kj} x_k} \right) \quad (9)$$

with

$$\tau_{ij} = \frac{g_{ij} - g_{ii}}{RT} \quad G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$$

UNIQUAC equation:

$$\begin{aligned} \ln \gamma_i &= \ln \gamma_i^C + \ln \gamma_i^R & (10) \\ \ln \gamma_i^C &= 1 - J_i + \ln J_i - 5q_i \left(1 - \frac{J_i}{L_i} + \ln \frac{J_i}{L_i}\right) \\ \ln \gamma_i^R &= q_i \left(1 - \ln S_i - \sum_j \theta_j \frac{\tau_{ij}}{S_j}\right) \end{aligned}$$

with

$$\begin{aligned} J_i &= \frac{r_i}{\sum_j r_j x_j} & L_i &= \frac{q_i}{\sum_j q_j x_j} & S_i &= \sum_l \theta_l \tau_{li} \\ \theta_i &= \frac{x_i q_i}{\sum_j x_j q_j} & \tau_{ij} &= \exp\left(-\frac{u_{ij} - u_{ii}}{RT}\right) \end{aligned}$$

The *FP* data for {2,2,4-trimethylpentane (1) + methylcyclohexane (2)}, {2,2,4-trimethylpentane (1) + ethylbenzene (2)}, and {2,2,4-trimethylpentane (1) + *p*-xylene (2)} mixtures were determined over the entire composition range. The optimized binary parameters for the Wilson, NRTL and UNIQUAC model used to estimate the activity coefficients were taken from literature references and are provided in Table 3 [24-25].

Table 3. The optimized binary parameters of the Wilson, NRTL and UNIQUAC equations for each binary system

Systems	Wilson		NRTL			UNIQUAC	
	A_{12} /J mol ⁻¹	A_{21} /J mol ⁻¹	A_{12} /J mol ⁻¹	A_{21} /J mol ⁻¹	α	A_{12} /J mol ⁻¹	A_{21} /J mol ⁻¹
{2,2,4-trimethylpentane (1) + methylcyclohexane (2)} ^a	218.030	-9.060	1.580	75.450	0.3	-1.260	-1.220
{2,2,4-trimethylpentane (1) + ethylbenzene (2)} ^b	607.303	537.921	-669.036	1842.650	0.4	176.547	13.215
{2,2,4-trimethylpentane (1) + <i>p</i> -xylene (2)} ^b	181.016	803.464	-72.834	1056.322	0.4	105.981	63.143

^a Ref. [24], ^b Ref. [25]

The optimized binary parameter is provided for the system {2,2,4-trimethylpentane (1) + methylcyclohexane (2)} from VLE data of the literature [24]. And the NRTL and UNIQUAC parameters are provided for the systems {2,2,4-trimethylpentane (1) + ethylbenzene (2)} and {2,2,4-trimethylpentane (1) + *p*-xylene (2)} in Ref. [25], thus the parameters of Wilson model were also made in this work.

The experimental binary *FP* data for the systems {2,2,4-trimethylpentane (1) + methylcyclohexane (2)}, {2,2,4-trimethylpentane (1) + ethylbenzene (2)} and {2,2,4-trimethylpentane (1) + *p*-xylene (2)} are presented in Table 4. The resulting binary data were compared with the predicted values from the activity coefficient models of Wilson, NRTL and UNIQUAC models.

The resulting binary data were compared with the predicted values from the activity coefficient models of the Wilson, NRTL, and UNIQUAC models. The binary parameters of each model equation were used to calculate the activity coefficients under the same conditions used in the experiments, and the initial temperature was assigned the numerical average temperature of each mixture. Subsequently, the *FP* was obtained by adjusting the initial temperature by satisfying Le Chatelier's rule (Equation 4). The objective function (*OF*) used is expressed as follows:

$$OF = \min \left[\left(\sum_i \frac{x_i \gamma_i P_i^{sat}}{P_{i,FP}^{sat}} \right) - 1 \right] \quad (10)$$

For Raoult's law, the activity coefficient was equal to unity based on the assumption of an ideal liquid phase. The average absolute deviations (*A.A.D*) between the experimental and calculated values are shown in Table 4.

The *A.A.D* is defined as follows:

$$A.A.D = \sum_{i=1}^N \frac{|T_i^{\text{exp}} - T_i^{\text{cal}}|}{N} \quad (11)$$

where the T_i^{exp} is the experimental lower *FP* of component *i*, and T_i^{cal} is the estimated lower flash point of component *i*.

The experimental data from the analysis of each binary system at 101.3 kPa are plotted in Figures 1 to 4. As shown from the minimum values of *A.A.D*, in all cases, the experimental data agree well with the predicted values. In addition, minimum flash point behavior (*MFPB*) was not observed in any of the three binary systems. The proposed approach for predicting the *FP* of aromatic hydrocarbon blends with 2,2,4-trimethylpentane proved to be accurate, having low deviations over almost the entire range of mixture compositions. For the investigated systems, the *A.A.D* values between the predicted and measured *FP* values were less than 1.99 K, except when calculated by Raoult's law. The Wilson model yielded results closest to those of the experimentally determined binary systems {2,2,4-trimethylpentane (1) + methylcyclohexane (2)} and {2,2,4-trimethylpentane (1) + *p*-xylene (2)}. The minimum

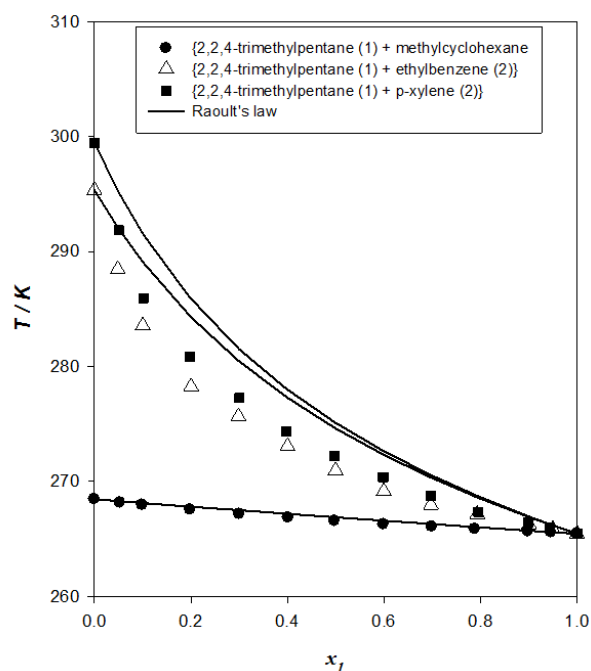


Figure 1. The comparison of the flash point prediction curves with the experimental data for the binary system at 101.3 kPa. Solid lines were calculated from Raoult's law.

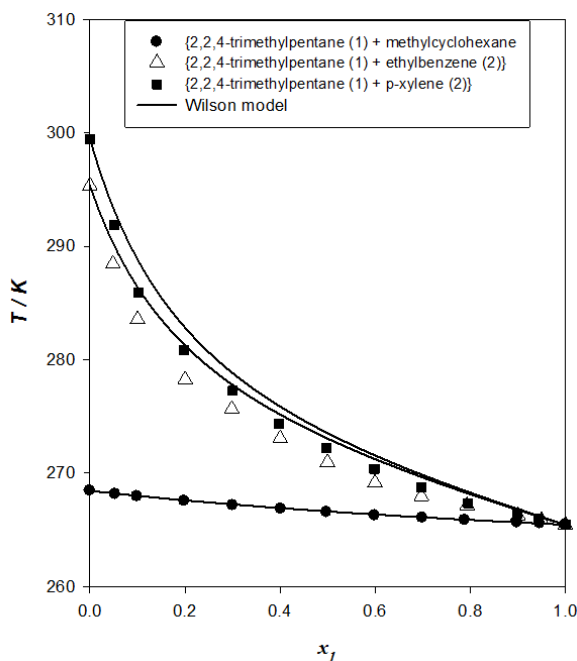


Figure 2. The comparison of the flash point prediction curves with the experimental data for the binary system at 101.3 kPa. Solid lines were calculated from Wilson model.

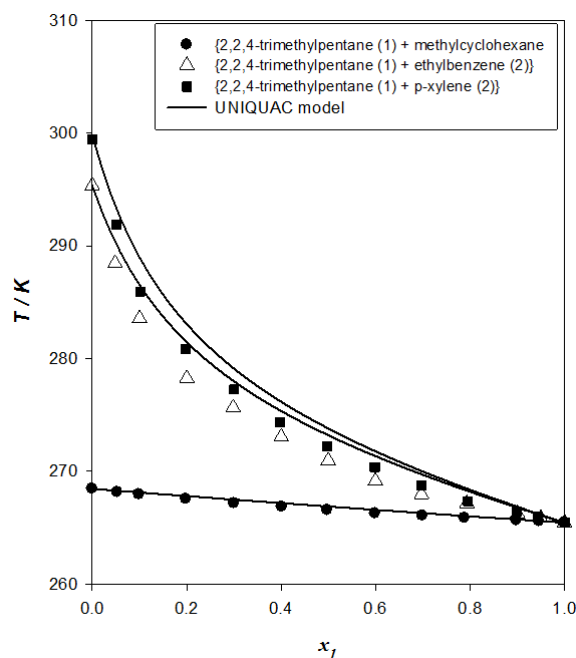


Figure 4. The comparison of the flash point prediction curves with the experimental data for the binary system at 101.3 kPa. Solid lines were calculated from UNIQUAC model.

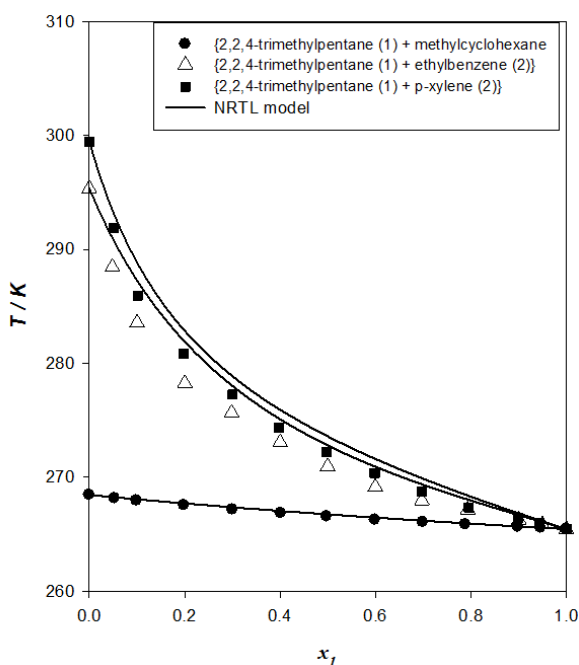


Figure 3. The comparison of the flash point prediction curves with the experimental data for the binary system at 101.3 kPa. Solid lines were calculated from NRTL model.

A.A.D values for the Wilson model are 0.06 and 1.35 K for {2,2,4-trimethylpentane (1) + methylcyclohexane (2)} and {2,2,4-trimethylpentane (1) + *p*-xylene (2)}, respectively. In the case of {2,2,4-trimethylpentane (1) + ethylbenzene (2)}, the minimum *A.A.D* calculated using the UNIQUAC model was 1.77 K. For the system {2,2,4-trimethylpentane (1) + methylcyclohexane (2)},

FP of each pure component is close (even the same value in the literature [15]), and slightly *FP*s were observed in the mixture than they expected.

The predicted data were only adequate for data determined by the closed-cup test method and may not be appropriate for data obtained from the open-cup test method because of its deviation from VLE. The predicted results of this work can be applied to design safe petrochemical processes, such as the identification of safe storage conditions for non-ideal solutions containing flammable components.

4. Conclusions

The lower *FP* data for {2,2,4-trimethylpentane + methylcyclohexane}, {2,2,4-trimethylpentane + ethylbenzene}, and {2,2,4-trimethylpentane + *p*-xylene} at 101.3 kPa were analytically determined using a SETA closed-cup flash point tester. *MFPB* was not observed in any binary system. The measured *FP* data agree well with the predicted values derived from the activity coefficient (G^E) models, i.e., Wilson, NRTL and UNIQUAC. The non-ideality of the mixture was also considered. Comparing the models, the Wilson model provided better results for the {2,2,4-trimethylpentane + methylcyclohexane} and {2,2,4-trimethylpentane + *p*-xylene} binary systems, whereas the UNIQUAC model gave slightly better prediction results for the {2,2,4-trimethylpentane + ethylbenzene} mixture.

Table 4. The experimental and predicted *F*Ps for each binary system at 101.3 kPa

Mole fractions	Flash points (K)				
	Exp.	Raoult's law	Wilson	NRTL	UNIQUAC
{2,2,4-trimethylpentane (1) + methylcyclohexane (2)}					
0.0000	268.45	-	-	-	-
0.0534	268.15	268.29	268.20	268.26	268.29
0.0993	267.95	268.12	268.00	268.06	268.12
0.1985	267.55	267.80	267.61	267.70	267.80
0.3005	267.15	267.50	267.24	267.37	267.49
0.4018	266.85	267.18	266.91	267.05	267.18
0.4976	266.55	266.88	266.63	266.74	266.88
0.5990	266.25	266.59	266.36	266.46	266.58
0.6997	266.05	266.30	266.10	266.19	266.30
0.7884	265.85	266.03	265.90	265.95	266.03
0.8987	265.65	265.72	265.66	265.68	265.72
0.9468	265.55	265.59	265.56	265.57	265.59
1.0000	265.45	-	-	-	-
<i>A.A.D</i>	-	0.22	0.06	0.14	0.22
{2,2,4-trimethylpentane (1) + ethylbenzene (2)}					
0.0000	295.35	-	-	-	-
0.0485	288.45	292.10	290.29	290.39	290.18
0.1003	283.55	289.09	286.38	286.57	286.27
0.2004	278.25	284.28	281.24	281.55	281.17
0.2985	275.65	280.50	277.82	278.18	277.80
0.4000	273.05	277.28	275.17	275.51	275.17
0.4998	270.95	274.61	273.05	273.36	273.07
0.5995	269.15	272.31	271.24	271.48	271.26
0.6971	267.95	270.34	269.66	269.83	269.68
0.7934	267.15	268.61	268.24	268.34	268.25
0.9005	266.25	266.89	266.75	266.79	266.76
0.9499	265.85	266.16	266.10	266.12	266.10
1.0000	265.45	-	-	-	-
<i>A.A.D</i>	-	3.26	1.79	1.99	1.77
{2,2,4-trimethylpentane (1) + <i>p</i> -xylene (2)}					
0.0000	299.45	-	-	-	-
0.0504	291.85	295.14	293.24	293.43	293.16
0.1014	285.95	291.49	288.74	288.83	288.58
0.1969	280.85	286.03	282.97	282.84	282.90
0.3003	277.25	281.49	278.81	278.92	278.86
0.3976	274.35	278.07	275.93	275.93	276.05
0.4977	272.25	275.15	273.57	273.59	273.71
0.5982	270.35	272.66	271.59	271.62	271.72
0.6965	268.75	270.56	269.89	269.92	269.99
0.7957	267.35	268.69	268.34	268.40	268.40
0.8985	266.45	266.97	266.85	266.83	266.87
0.9430	265.95	266.28	266.23	266.14	266.24
1.0000	265.45	-	-	-	-
<i>A.A.D</i>	-	2.83	1.35	1.37	1.37

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