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VAPOUR-LIQUID EQUILIBRIUM IN SYSTEMS WITH ISOBUTYL ACETATE, ACETIC ACID AND METHYL ETHYL KETONE

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The experimental temperature dependence of the vapour pressures of isobutyl acetate, acetic acid and methyl ethyl ketone were determined, and isobaric vapour–liquid equilibrium data of binary systems of methyl ethyl ketone + isobutyl acetate and methyl ethyl ketone + acetic acid were obtained. The experimental data were processed using the Antoine and Riedel equations and the NRTL and Wilson local composition equations, respectively. Comparison of the experimental and calculated data confirmed the adequacy of the vapour–liquid equilibrium mathematical simulation.

Ключевые слова: *vapour–liquid equilibrium, vapour pressure, mathematical simulation, isobutyl acetate, acetic acid, methyl ethyl ketone.*

ПАРОЖИДКОСТНОЕ РАВНОВЕСИЕ В СИСТЕМАХ, СОДЕРЖАЩИХ ИЗОБУТИЛАЦЕТАТ, УКСУСНУЮ КИСЛОТУ, МЕТИЛЭТИЛКЕТОН

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В натурном эксперименте определены зависимости упругости паров изобутилацетата, уксусной кислоты, метилэтилкетона, равновесные температуры кипения и составы паровой фазы в системах изобутилацетат – метилэтилкетон и уксусная кислота – метилэтилкетон при атмосферном давлении. Опытные данные обработаны, соответственно, уравнениями Антуана и Риделя, уравнениями локальных составов NRTL и Вильсон. Сравнение расчетных и экспериментальных данных подтвердило адекватность математического моделирования парожидкостного равновесия.

Keywords: *парожидкостное равновесие, упругость пара, моделирование, изобутилацетат, уксусная кислота, метилэтилкетон.*

Introduction

Reliable experimental data on the vapour–liquid equilibrium (VLE) of binary systems are necessary to obtain adequate mathematical parameters, which enable one to investigate the phase equilibrium and estimate optimal operation parameters of single distillation columns and the entire flow sheet.

The ternary system of isobutyl acetate (IBA) + acetic acid (AA) + methyl ethyl ketone (MEK) is notably interesting, because it includes the binary IBA+AA system with two binary azeotropes [1, 2]. Its separability in the presence of MEK by extractive distillation has been argued by Chelyuskina et al. [3].

In the present article, the IBA+AA+MEK ternary system was selected as an object of phase-diagram study. There are no experimental VLE data of the binary MEK+IBA system [4, 5].

The investigation of VLE of the ternary IBA+AA+MEK system is necessary to determine the NRTL and Wilson binary interaction parameters and to design the separation processes.

Experimental (Chemicals, Apparatus and Procedure)

In the first step of experimental research, MEK (Hungarian manufacturer, qualification: “for electrotechnical purpose”), IBA (Belgian manufacturer, 98% mass), and AA (Russian manufacturer, qualification: “chemically pure”) were purified, because there were relatively small amounts of impurities (up to 1% by weight in MEK and IBA and up to 1.5% in AA). The impurities were identified using gas-liquid chromatography.

MEK was dried on molecular sieves (3 Å), which were heated to 693.15 K. The concentration of MEK after purification was 99.9% by mass.

IBA was purified from AA impurities by adding dry alkali (KOH). IBA was boiled at reflux for 6 hours. The splitting distillate was selected, its organic phase (IBA) was dried on molecular sieves, and the water phase was used. The purity of IBA was more than 99.9% by mass.

AA was purified using a packed batch distillation column, which was filled with a Fenske glass nozzle. The efficiency of the packed column was approximately 15 theoretical stages. The concentration of AA after purification was 99.95% by mass.

For MEK, IBA and the MEK+IBA binary mixture, the conditions of the GC analysis were as follows: packed column, 10% chlorosilicone XC-2-1 on Polychrom-1; column material, stainless steel; column length, 2.5 m; internal diameter, 4 mm; carrier gas, helium; carrier gas volume rate, 100 mL/min; thermal conductivity detector; column temperature, $t_{col} = 80°C$; evaporator temperature, $t_{ev} = 250°C$; detector temperature, $t_d = 150°C$; detector amperage, $i_d = 150$ mA.

For the AA component and the MEK+AA mixture, the conditions of the GC analysis were as follows: packed column, 10% polyphenylmethylsiloxane on Polychrom-1; column material, glass; column length, 3.0 m; internal diameter, 4 mm; carrier gas, helium; carrier gas volume rate, 100 mL/min; thermal conductivity detector; $t_{co\,l} = 90°C$; $t_{ev} = 250°C$; $t_d = 150°C$; $i_d = 150$ mA.

The outlet order of the components on the chromatograms was MEK-IBA and then MEK-AA. In the method of internal normalization [6], MEK was used as the linking component (its correction coefficient is 1). The correction coefficients for the other components of the binary mixture were 0.7826 for IBA and 0.8012 for AA. The uncertainty in mass fraction was less than 3%.

The physical-chemical properties of the components are provided in Table 1.

Table 1. Physical-chemical properties of the components

Component	Properties		
	n_D^{20}, refraction index	ρ_4^{20}, density, g/cm^3	Boiling point, K at 101.33 kPa
MEK	1.3784	0.8046	352.45
IBA	1.3900	0.8705	391.15
AA	1.3718	1.0495	390.95

Experimental investigation of the VLE was performed using a modified Sventoslavsky’s [7] still. The construction of the still enables one to pick a sample of vapour using a 1-2 mkL chromatographic syringe without interrupting the experiment.

The VLE measurements were performed at 101.33 kPa azeotropes; the pressure was maintained using an electronic system with an accuracy of ±0.5 kPa. The temperature was measured using a calibrated thermocouple, which was inserted in a thermometric sleeve filled with glycerol; the accuracy was 0.1°C. The samples of vapour condensate were analysed using the GC method. The vapour pressure was determined using a modified Sventoslavsky’s still.

Results and Discussion

Determination of the vapour pressures of the components

The experimental values of vapour pressure of the pure components are provided in Table 2. The experimental dependences of the vapour pressure on temperature were described using Antoine (1) and Riedel (2) equations:

$$Ln(P^s) = a - b/(c+T) \tag{1}$$

$$Ln(P^s) = A + B/T + CLn(T) + DT^2 \tag{2}$$

where P^s is in mm Hg and T is in K.

The coefficients of the equations were evaluated using experimental data and are provided in Table 3.

Because the units of pressure in the experiment and equations (1) and (2) are mm Hg, the values of the component vapour pressures in Table 2 have the same units.

The comparison of the calculated and experimental vapour pressures (Table 2) demonstrates the satisfactory description of experimental data using both equations. The average deviations of the calculated values obtained using both equations are similar. However, there is an increase in the relative deviation in the series of components of ketone–ester–acid, which may be related to the peculiarity of a molecular interaction.

Table 2. Vapour pressure of the components (mm Hg)

T, K	P^s, mm Hg	Calculation by Eq. No.		Absolute deviation		Relative deviation, %	
		(1)	(2)	Eq. No. (1)	Eq. No. (2)	Eq. No. (1)	Eq. No. (2)
MEK							
302.62	100	100.3	100.8	-0.3	-0.8	-0.3	-0.8
310.33	150	149.0	148.7	1.0	1.3	0.67	0.87
316.57	200	199.9	199.0	0.1	1.0	0.05	0.50
321.76	250	251.2	250.0	-1.2	0.0	-0.48	0.00
326.20	300	302.1	300.8	-2.1	-0.8	-0.70	-0.27
330.09	350	352.6	351.2	-2.6	-1.2	-0.74	-0.34
333.60	400	403.0	401.7	-3.0	-1.7	-0.75	-0.43
336.75	450	452.4	451.4	-2.4	-1.4	-0.53	-0.31
339.65	500	501.6	500.8	-1.6	-0.8	-0.32	-0.16
342.36	550	550.8	550.3	-0.8	-0.3	-0.15	-0.05
344.91	600	600.1	599.8	-0.1	0.2	-0.02	0.03
347.30	650	649.0	649.0	1.0	1.0	0.15	0.15
349.61	700	698.8	699.1	1.2	0.9	0.17	0.13
352.45	760	763.5	764.2	-3.5	-4.2	-0.46	-0.55
average deviation module				*1.5*	*1.1*	*0.39*	*0.33*
IBA							
325.13	62	63.2	62.7	-1.2	-0.7	-1.93	-1.16
333.65	101	99.9	99.1	1.1	1.9	1.05	1.87
342.15	151	149.5	149.1	1.5	1.9	1.01	1.23
348.87	201	198.9	199.7	2.1	1.3	1.04	0.65
354.47	251	247.6	249.8	3.4	1.2	1.35	0.48
361.05	320	314.1	318.1	5.9	1.9	1.84	0.59
367.33	401	387.4	392.6	13.6	8.4	3.39	2.09
372.06	470	449.1	454.5	20.9	15.5	4.44	3.29
379.75	550	561.7	564.5	-11.7	-14.5	-2.13	-2.64
384.54	620	639.6	638.1	-19.6	-18.1	-3.16	-2.92
388.13	690	702.0	695.3	-12.0	-5.3	-1.74	-0.77
391.15	760	757.1	744.5	2.9	15.5	0.38	2.04
average deviation module				*8.0*	*7.2*	*1.96*	*1.64*
AA							
321.63	52	53.5	52.0	-1.5	0.0	-2.88	0.00
326.63	67	67.8	66.3	-0.8	0.7	-1.19	1.19
334.92	96	98.7	97.2	-2.7	-1.2	-2.81	-1.25
341.25	127	129.4	128.4	-2.4	-1.4	-1.89	-1.10
345.95	156	157.1	156.7	-1.1	-0.7	-0.71	-0.45
351.92	199	199.1	199.9	-0.1	-0.9	-0.05	-0.45
357.72	246	248.3	251.1	-2.3	-5.1	-0.94	-2.07
365.25	337	326.6	333.3	10.4	3.7	3.09	1.10
368.15	375	361.7	370.4	13.3	4.6	3.55	1.23
373.25	449	430.7	444.0	18.3	5.0	4.08	1.11
376.15	512	474.5	490.9	37.5	21.1	7.32	4.12
379.35	571	527.0	547.3	44.0	23.7	7.71	4.15
383.15	634	595.2	621.0	38.8	13.0	6.12	2.05
388.25	698	697.7	732.6	0.3	-34.6	0.04	-4.96
390.95	760	757.5	798.0	2.5	-38.0	0.33	-5.00
average deviation module				*11.7*	*10.2*	*2.85*	*2.02*

Table 3. Coefficients of the equations used to calculate the vapour pressures of the components

Coefficients	MEK	IBA	AA
Antoine equation (1)			
A	12.8913	11.3360	16.5511
B	1271.51	899.651	3262.07
C	-149.12	-200.00	-62.15
Riedel equation (2)			
A	239.919	232.688	68.7142
B	-13794.7	-18923.6	-7210.7
C	-33.5537	-39.8283	-7.4069
D	$2.13199 \cdot 10^{-5}$	$2.78852 \cdot 10^{-7}$	$4.06060 \cdot 10^{-6}$

Table 4. Experimental VLE data for binary systems at 101.33 kPa

Point No.	MEK mole fraction		Boiling point, °C
	liquid, *x*	vapour, *y*	
MEK+IBA system			
1	0.9254	0.9735	80.7
2	0.8866	0.9570	81.6
3	0.7957	0.9237	83.8
4	0.7338	0.8988	85.35
5	0.6732	0.8675	87.00
6	0.6118	0.8282	88.8
7	0.5565	0.7808	90.5
8	0.5178	0.7702	91.7
9	0.4725	0.7351	93.2
10	0.4238	0.7028	94.9
11	0.3641	0.6396	97.6
12	0.3055	0.5695	101.0
13	0.2606	0.5240	102.9
14	0.2160	0.4433	104.8
15	0.1752	0.3859	106.7
16	0.1626	0.3510	107.4
17	0.1210	0.2974	109.5
18	0.0895	0.2250	111.8
MEK+AA system			
1	0.0265	0.0794	116.10
2	0.0440	0.1125	115.20
3	0.1005	0.1998	112.30
4	0.1324	0.2762	110.60
5	0.2720	0.5060	104.20
6	0.3526	0.6085	101.00
7	0.4358	0.7201	97.20
8	0.5330	0.8082	93.50
9	0.6356	0.8718	90.40
10	0.7610	0.9400	86.40
11	0.8916	0.9836	82.50
12	0.9564	0.9960	80.60

Experimental VLE data and thermodynamical consistency test

The experimental VLE data for the MEK+IBA (18 points) and MEK+AA (12 points) systems are provided in Table 4.

In the following stage, the experimental VLE data were verified for thermodynamic consistency. The test was performed using the Herringtone and Redlich-Kister criteria [5, 8]. The vapour pressure was calculated using the Riedel equation (2). The graphical processing of the results for the MEK+IBA system is shown in Figure 1.

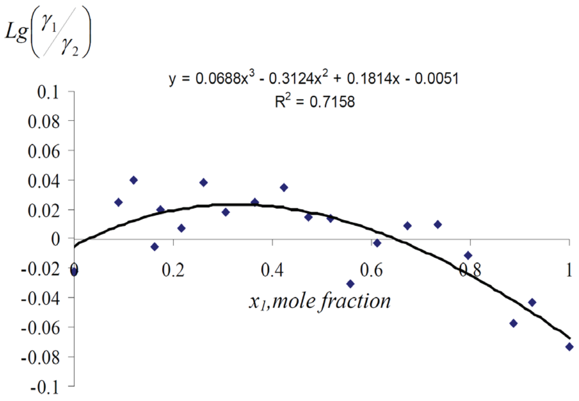

Fig. 1. Dependence of the logarithm of the ratio of activity coefficients of MEK (1) and IBA (2) on the composition.

The dependence of the logarithm of the ratio of activity coefficients was approximated in Microsoft Excel using a cubic polynomial. By integrating this curve in a mole fraction range (0–1) we determined the value of the Herringtone and Redlich-Kister criterion to be -0.0013, which is in the range of permissible values ±0.02 [5]. Thus, the obtained experimental VLE data for the MEK+IBA system are thermodynamically consistent.

For the MEK+AA system, the thermodynamic consistency test was conducted regarding the non-ideality of the vapour phase in the virial equation. The liquid mole volumes were calculated from the density data [9] at an average temperature of 99.1°C for the experimental data (Table 4). This value was 0.1012 L/mol for MEK and -0.0626 L/mol for AA.

The second virial coefficients of AA were graphically interpolated from the experimental data in [5]. The second virial coefficients for MEK and cross coefficients were calculated using the Pitzer and Curl method [9]. The results for the MEK+AA system are shown in Figure 2.

The dependence of Lg(γ_1/γ_2) was approximated in Microsoft Excel using a 5th-order polynomial.

By integrating the curve in Figure 2 we obtain a Herringtone and Redlich-Kister criterion of 0.008. This value is in the permissible range ±0.02; therefore, the experimental VLE data for the MEK+AA system are thermodynamically consistent.

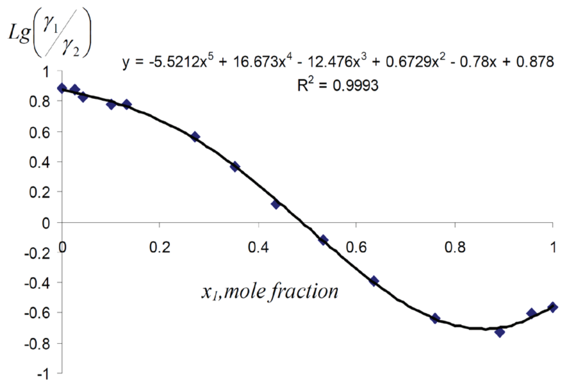

Fig. 2. Dependence of the logarithm of the ratio of activity coefficients of MEK (1) and AA (2) on the composition.

Mathematical simulation of the vapour–liquid equilibrium

The vapour-liquid equilibrium in binary systems was modelled using NRTL and Wilson models as follows:

NRTL [10]:

$$\ln\gamma_i = \frac{\sum\limits_j x_i\tau_{ji}G_{ji}}{\sum\limits_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum\limits_k x_k G_{kj}}\left(\tau_{ij} - \frac{\sum\limits_m x_m\tau_{mj}G_{mj}}{\sum\limits_k x_k G_{kj}}\right) \qquad (3)$$

where $G_{ij} = \exp(-\alpha_{ij}\tau_{il})$;

$\tau_{ij} = \alpha_{ij} + \frac{b_{ij}}{T} + e_{ij}\ln T + f_{ij}T$;

$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15K)$;

$\tau_{ii} = 0$;

$G_{ii} = 1$.

Wilson [11]:

$$\ln\gamma_i = 1 - \ln\left(\sum_j A_{ij}x_j\right) - \sum_j \frac{A_{ij}x_j}{\sum\limits_k A_{jk}x_k}\ , \qquad (4)$$

where $\ln A_{ij} = a_{ij} + \frac{b_{ij}}{T} + c_{ij}\ln T + d_{ij}T + \frac{e_{ij}}{T^2}$

The binary interaction parameters of the Wilson and NRTL models were obtained using experimental VLE data (Tables 5 and 6).

The boiling points and equilibrium vapour compositions in the considered systems were calculated on the basis of two local-composition equations and two vapour pressure equations. The calculations were performed with the use of the Flash unit operation in Aspen Plus. The considered pressure was 101.33 kPa.

Thus, for each binary system, four sets of calculated

Table 5. Wilson parameters

Equation for P^s(T)	B_{12}, K	B_{21}, K
MEK (1) + IBA (2) System		
Antoine	231.4381	-81.91546
Riedel	201.2251	-71.70725
MEK (1) +AA (2) System		
Antoine	73.85846	-44.98935
Riedel	-486.7422	604.5862

Table 6. NRTL parameters

Equation for P^s(T)	B_{12}, K	B_{21}, K	α
MEK (1) + IBA (2) System			
Antoine	533.608	-359.509	0.2716
Riedel	348.975	-232.443	0.4000
MEK (1) + AA (2) System			
Antoine	-815.901	1046.739	0.107249
Riedel	-26.8003	-1608.93	-1.20565

VLE data with different combinations of the Wilson and NRTL equation and the Antoine and Riedel equations were obtained (Table 7).

The VLE data are well described by both Wilson and NRTL equations. For the MEK+IBA system, the lowest average relative deviations are observed with the combination of the Wilson and Antoine equations. For this system, the Antoine and Riedel equation can be used to calculate the vapour pressure. For the MEK+AA system, the equation combinations Wilson+Riedel, NRTL+Antoine, NRTL+Riedel can be used. All combinations give a satisfactory correspondence between experimental and calculated VLE data. However, the average deviations in this case are higher than in previous cases, which may be related to the non-ideality of the vapour phase.

Table 7. Comparative analysis of the calculated VLE data at 101.33 kPa

Set of calculated VLE data	Equation for VLE calculation		Equation for P^s(T)		Average rel. dev., %	
					Δy_1	Δt
MEK+IBA System						
1	Wilson	-	Antoine	-	**0.98**	**0.20**
2	Wilson	-	-	Riedel	2.23	0.24
3	-	NRTL	Antoine	-	1.75	0.20
4	-	NRTL	-	Riedel	1.72	0.24
MEK+AA System						
5	Wilson	-	Antoine	-	4.19	0.56
6	Wilson	-	-	Riedel	**3.90**	0.48
7	-	NRTL	Antoine	-	4.28	**0.24**
8	-	NRTL	-	Riedel	5.32	0.37

It should be noted that the NRTL binary-interaction parameters, which were obtained on the basis of the presented experimental data, may be useful for the simulation of the phase equilibrium of multicomponent multiphase systems, which contain the binary mixtures MEK+IBA, MEK+AA and water, for example.

The calculated VLE data for the equation combinations, which correspond to set 1 for the MEK+IBA system and sets 6–7 for the MEK+AA system, are characterized by lower average deviations, as shown in Tables 8–10.

Conclusion

Experimental data were obtained for the temperature dependence of the vapour pressure of isobutyl acetate, methyl ethyl ketone, acetic acid and vapour–liquid equilibrium data for the binary MEK+IBA and MEK+AA systems at 101.33 kPa. By combining the Wilson and NRTL equations with the Antoine and Riedel equations, eight sets of the calculated VLE data for the binary MEK+IBA and MEK+AA systems were obtained. All calculated data are consistent with the experimental data.

Table 8. Calculated VLE data for the MEK (1)+IBA (2) system at 101.33 kPa. Wilson+Antoine equations

Liquid mole fraction x_1	Calculation		Deviations			
	y_1, mole fr.	t, ^{0}C	Δy_1		Δt	
			abs., mole fr.	rel., %	abs., °C	rel., %
1	1.0000	79.15	0.0000	0.00	0.15	0.19
0.9254	0.9734	80.73	-0.0001	-0.38	-0.03	-0.03
0.8866	0.9593	81.58	0.0023	5.35	0.02	0.03
0.7957	0.9238	83.70	0.0001	0.13	0.08	0.09
0.7338	0.8967	85.28	-0.0021	-2.08	0.07	0.09
0.6732	0.8669	86.94	-0.0006	-0.45	0.06	0.07
0.6118	0.8329	88.75	0.0047	2.74	0.03	0.03
0.5565	0.7982	90.51	0.0174	7.94	-0.06	-0.07
0.5178	0.7707	91.85	0.0005	0.22	-0.17	-0.19
0.4725	0.7368	93.44	0.0017	0.64	-0.23	-0.25
0.4238	0.6954	95.28	-0.0074	-2.49	-0.34	-0.36
0.3641	0.6376	97.71	-0.0020	-0.55	-0.11	-0.11
0.3055	0.5721	100.30	0.0026	0.60	0.72	0.72
0.2606	0.5150	102.42	-0.0090	-1.89	0.51	0.49
0.2160	0.4513	104.68	0.0080	1.44	0.14	0.14
0.1752	0.3859	106.87	0.0000	0.00	-0.14	-0.13
0.1626	0.3642	107.58	0.0132	2.03	-0.20	-0.18
0.1210	0.2869	110.01	-0.0105	-1.49	-0.51	-0.47
0.0895	0.2220	111.97	-0.0030	-0.39	-0.15	-0.13
0	1.0000	118.16	0.0000	0.00	-0.16	-0.13
average deviation			*0.0047*	*1.71*	*0.19*	*0.20*

Table 9. Calculated VLE data for the MEK (1) + AA (2) system at 101.33 kPa. Wilson + Riedel equations

Liquid mole fraction x_1	Calculation		Deviations			
	y_1, mole fr.	t, ^{0}C	Δy_1		Δt	
			abs., mole fr.	rel., %	abs., °C	rel., %
0	0.0000	116.26	0.0000	0.00	1.54	1.31
0.0265	0.0626	115.08	0.0168	9.07	1.02	0.88
0.0440	0.1023	114.29	0.0102	-11.01	0.91	0.79
0.1005	0.2218	111.78	-0.0220	-2.72	0.54	0.48
0.1324	0.2837	110.36	-0.0075	-1.19	0.24	0.22
0.2720	0.5120	104.31	-0.0060	-1.22	-0.11	-0.11
0.3526	0.6159	100.94	-0.0074	2.07	0.06	0.06
0.4358	0.7052	97.58	0.0149	1.37	-0.38	-0.39
0.5330	0.7898	93.83	0.0110	1.34	-0.33	-0.35
0.6356	0.8601	90.11	0.0117	1.66	0.29	0.32
0.7610	0.9244	85.91	0.0156	1.20	0.49	0.57
0.8916	0.9718	82.00	0.0118	0.64	0.50	0.61
0.9564	0.9896	80.25	0.0064	9.07	0.35	0.43
1	1.0000	79.13	0.0000	0.00	0.17	0.21
average deviation			*0.0101*	*3.90*	*0.50*	*0.48*

The lowest average relative deviations of the vapour composition and boiling point description are observed in the following cases: the MEK+IBA system with the Wilson and Antoine equations (Δy_1, Δt); the MEK+AA system with the Wilson and Riedel equations (Δy_1,) and the NRTL and Antoine equations (Δt).

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Table 10. Calculated VLE data for the MEK (1) + AA (2) system at 101.33 kPa. NRTL + Antoine equations

Liquid mole fraction x_1	Calculation		Deviations			
	y_1, mole fr.	t, °C	Δy_1		Δt	
			abs., mole fr.	rel., %	abs., °C	rel., %
0	0.0000	117.91	0.0000	0.00	-0.11	-0.09
0.0265	0.0732	116.28	0.0062	7.75	-0.18	-0.16
0.0440	0.1177	115.26	-0.0052	-4.60	-0.06	-0.05
0.1005	0.2439	112.17	-0.0441	-22.09	0.15	0.13
0.1324	0.3059	110.56	-0.0297	-10.75	0.04	0.04
0.2720	0.5232	104.17	-0.0172	-3.40	0.03	0.02
0.3526	0.6205	100.82	-0.0120	-1.97	0.18	0.18
0.4358	0.7051	97.51	0.0150	2.08	-0.31	-0.32
0.5330	0.7871	93.83	0.0137	1.71	-0.33	-0.36
0.6356	0.8568	90.15	0.0150	1.73	0.25	0.27
0.7610	0.9220	85.97	0.0180	1.92	0.43	0.49
0.8916	0.9709	82.04	0.0127	1.29	0.46	0.55
0.9564	0.9894	80.27	0.0066	0.66	0.33	0.40
1	1.0000	79.15	0.0000	0.00	0.18	0.23
average deviation			*0.0139*	*4.28*	*0.22*	*0.24*

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