

SELECTED DATA ON MIXTURES

International Data Series*

3. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3028

Compiled by Thermodynamics Research Center

Components: 1. Methylcyclohexane, C₇H₁₂ [57-55-1]
2. Methyl ethanoate, C₃H₆O₂ [79-20-9]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature
x_i, mole fraction of component i in liquid phase
y_i, mole fraction of component i in vapor phase
P, pressure

Parameters: P, pressure

Method: Direct measurement of T, x_i and y_i at constant P; ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

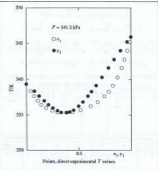
Edited by: Szwarc, A., Mijczyk, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Blasso, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P = 141.3						
x ₁	ZK	y ₁	x ₂	ZK	y ₂	
0.000	339.30	0.000	0.903	344.83	0.908	
0.041	336.40	0.077	0.987	341.25	0.963	
0.074	337.71	0.122	1.000	343.92	1.000	
0.110	337.85	0.170				
0.142	336.47	0.231				
0.187	336.02	0.253				
0.248	335.66	0.297				
0.296	335.40	0.332				
0.386	335.37	0.381				
0.442	335.47	0.414				
0.517	335.75	0.450				
0.613	336.30	0.499				
0.679	336.89	0.540				
0.745	337.71	0.588				
0.785	338.35	0.622				
0.826	339.20	0.666				
0.870	340.35	0.722				
0.910	341.65	0.783				
0.937	342.79	0.836				



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebullimeter employing continuous circulation of the liquid and vapor phases with a charge capacity of 30 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebullimeter was connected to a vacuum pump and a Fisher model VK1 pressure controller. High purity nitrogen was used for the backing pressure. The temperatures were measured by an ASL-725 digital platinum resistance thermometer with a precision of readings ± 0.01 K.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ± 0.07 kg m⁻³. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition = 0.002 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland); degassed ultrasonically, dried over molecular sieves 3A.
2. Fluka AG (Buchs, St. Gallen, Switzerland); purity = 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; n_D²⁰ = 1.3588, ρ₂₀ = 828.15 kg m⁻³, T_b = 327.01, T_c = 505.52 (kPa/K) = 329.87.

Notes: [a]_D²⁰ = 0.01, [α]_D²⁰ = 200, [n]_D²⁰ = 0.002, [η]₂₅ = 0.91.

REFERENCES

1. Int. Data Ser., Ser. A, *Guidelines* 3B, 1994, 22(4).
2. Blasso, A. M.; Ortega, J. *J. Chem. Eng. Data*, 1996, 41, 566.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. *J. Chem. Eng. Data*, 1986, 31, 339.

JANUARY 31, 2003, Vol. 34, No. 1, pp. 1-11

SELECTED DATA ON MIXTURES
International DATA Series*

No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamic Research Center

Composities:	1. Methanol, CH ₃ O (67-56-1)
	2. Methyl ethanoate, C ₃ H ₆ O ₂ (79-20-9)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T, temperature
	x _i , mole fraction of component i in liquid phase
	y _i , mole fraction of component i in vapor phase
Parameters:	Z, pressure
Method:	Calculation from direct experimental liquid-vapor equilibrium temperatures, T _{exp} data at variable x ₁ and constant P, ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, de Iabte 36, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Orent, F. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

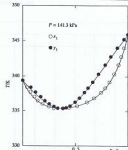
SOURCE OF DATA

Hiano, A. M.; Ortega, J. Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain; FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calculated values of y₁

P/MPa = 141.3		
x ₁	T/K	y ₁
0.00	338.38	0.0000
0.05	333.99	0.0879
0.10	331.04	0.1533
0.15	328.38	0.2092
0.20	325.50	0.2538
0.25	323.66	0.2919
0.30	322.50	0.3234
0.40	320.45	0.3837
0.50	318.70	0.4368
0.60	316.28	0.4914
0.70	315.16	0.5549
0.75	315.83	0.5933
0.80	316.68	0.6391
0.85	318.80	0.6935
0.90	341.27	0.7677
0.95	343.78	0.8644
1.00	345.92	1.0000

Standard deviation of T/K, relative standard deviation 100(ΔT/T), and absolute maximum deviation Δy₁/y₁ at P/MPa = 141.3 are resp. -0.94, 0.326, 0.201.



Points, direct experimental T values, cases, (x₁, y₁) and T(y₁), calculated from the equations.

EQUATIONS

$$G^E(T) = -x_1 \ln(x_1 + c_1 x_1^2) - x_2 \ln(x_2 + c_2 x_2^2)$$

$$v_1 = \exp\left[-(a_1 + \frac{a_1^2}{T})\right] \quad v_2 = \exp\left[-(a_2 + \frac{a_2^2}{T})\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^s \exp\left[\frac{v_i^L - (B_{ii} - V_i^L)P - P_i^s - 2P H_{ii}(1 - y_1)^2}{RT}\right]$$

$$P_i^s = G^S - x_i^L (G^S / dx_i)_{T,P} \quad P_i^s = G^S - x_i^V (G^S / dx_i)_{T,P}$$

$$B_{ii}^S = B_{ii}^L - (B_{ii}^L + B_{ii}^V)/2; y_1 = P/P^s; P^s/MPa = \exp(L_i + B_i/C_i + T/K)$$

COEFFICIENTS IN THE EQUATIONS

P/MPa	a ₁ /K	a ₂ /K ²	a ₁ /K ²	a ₂ /K ²
141.3	269.30	8	170.00	0
	(7.3)	(0)	(7.0)	(0)

The standard deviations (σ_{ai}) of the coefficients a_i are given in parentheses.

P/MPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
141.3	16.48182	-3567.81	-36.51	14.36391	-2662.70	-53.40

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 141.3 kPa are reported in ref. 2.

Computations: The 22 T_{exp} data at 141.3 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies μ_i^E.

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd order virial coefficients B_{ii}^S, ref. 5, and the molar volume under saturation pressure V_i^S, ref. 6.

Errors: Standard deviation of T = [(dT - T_{exp})<sup>2]/(N-2)]^{1/2}
Relative standard deviation 100(ΔT/T) = 100[(dT - T_{exp})<sup>2]/(N-2)]^{1/2}
N, number of experimental points, ref. 2.
n, number of coefficients in the smoothing equation.</sup></sup>

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- Ortega, J. *Int. DATA Ser., Ser. Data Mixtures*, Ser. A, 2003, IV, 10.
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- Thomson, G. *AIChE J.*, 1974, 20, 262, 1970, 21, 827.
- Yeo, L. C.; Woods, S. S. *AIChE J.*, 1966, 12, 95.

SELECTED DATA ON MIXTURES

International Data Series*

3. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80305-3328

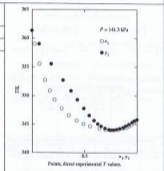
Compiled by Thermodynamics Research Center

Components:	1. Methanol, CH ₃ O (87-38-1) 2. Methyl propionate, C ₄ H ₈ O ₂ (754-12-1)
States:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T, temperature x _i , mole fraction of component i in liquid phase y _i , mole fraction of component i in vapor phase
Parameters:	P, pressure
Method:	Direct measurement of T, x _i and y _i at constant P; ref. 1

Author(s) of table:	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by:	Skowas, A.; Mazytycki, A.; Gierzycki, C. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
SOURCE OF DATA	
Blanco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2	

DIRECT EXPERIMENTAL VALUES

P/kPa = 141.3						
x ₁	T/K	y ₁	x ₂	T/K	y ₂	
0.000	361.38	0.000	0.950	363.06	0.929	
0.024	359.92	0.068	0.971	363.40	0.952	
0.070	355.55	0.383	0.985	363.70	0.974	
0.123	352.75	0.296	1.000	363.92	1.000	
0.169	350.89	0.371				
0.214	349.24	0.438				
0.282	347.85	0.490				
0.349	346.60	0.545				
0.423	345.73	0.598				
0.489	345.12	0.626				
0.552	344.72	0.658				
0.642	344.34	0.695				
0.699	344.12	0.732				
0.758	344.06	0.758				
0.782	344.06	0.775				
0.829	344.15	0.806				
0.868	344.32	0.835				
0.902	344.51	0.862				
0.927	344.79	0.894				



AUXILIARY INFORMATION

Apparatus:	The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm ³ ; ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and a Fisher model VEC pressure controller. High purity nitrogen was used for the backing pressure. The temperatures were measured by a ANL-F25 digital platinum resistance thermometer with a precision of readings ± 0.01 mK.
Procedure:	The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-35 ultrasonic-ruby digital densimeter with a precision of ± 0.02 kg m ⁻³ . A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition < 0.002 mole fraction.
Materials:	1. Fluka AG (Buchs, St. Gallen, Switzerland); degassed ultrasonically, dried over molecular sieves 3A. 2. Fluka AG (Buchs, St. Gallen, Switzerland); degassed ultrasonically, dried over molecular sieves 3A; $d(0, 298.15 \text{ K}) = 1.3745$, $d(298.15 \text{ K}) \text{ kg m}^{-3} = 989.35$, $T_b(0.02 \text{ kPa})/\text{K} = 351.35$.
Errors:	$ u(T) /\text{K} = 0.01$; $ u(P) /\text{kPa} = 200$; $ u(x_1) = 0.002$; $ u(y_1) = 0.01$.

REFERENCES

- Int. J. Ref. Data Ser., Ser. A, Goldsch. 36, 1994, 23(4).
- Blanco, A. M.; Ortega, J. *J. Chem. Eng. Data*, 1996, 41, 566.
- Ortega, J.; Peña, J. A.; de Abajo, C. *J. Chem. Eng. Data*, 1996, 41, 339.

10.1021-10.53031-1218

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Int. J. Ref. Data Ser., Ser. A, Goldsch. 36, 1994, 23(4)

SELECTED DATA ON MIXTURES
International Data Series*
36. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80501-3328

Compiled by Thermodynamic Research Center

Components: 1. Methanol, CH₃O (67-56-1)
2. Ethyl ethanoate, C₄H₈O₂ (141-78-6)

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature
x_i, mole fraction of component i in liquid phase
y_i, mole fraction of component i in vapor phase

Parameters: P, pressure

Method: Direct measurement of T, x_i and y_i at constant P, wt. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 3871 Las Palmas de Gran Canaria, Canary Islands, Spain)

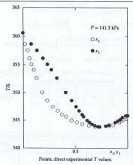
Edited by: Skrzysz, A.; Majczyk, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Hisco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), vol. 2

DIRECT EXPERIMENTAL VALUES

P/Pa = 141.3					
x ₁	TK	y ₁	x ₂	TK	y ₂
0.000	348.62	0.000	0.872	344.00	0.791
0.029	348.69	0.078	0.879	344.18	0.821
0.043	347.55	0.134	0.920	344.67	0.881
0.063	346.19	0.190	0.942	345.95	0.907
0.082	345.14	0.234	0.964	345.21	0.930
0.100	344.16	0.270	0.975	345.58	0.949
0.129	342.66	0.325	0.991	345.88	0.981
0.164	348.14	0.469	1.000	345.92	1.000
0.233	348.66	0.465			
0.285	347.51	0.506			
0.331	348.74	0.536			
0.371	348.05	0.565			
0.411	345.68	0.579			
0.464	345.02	0.612			
0.516	348.65	0.636			
0.566	344.32	0.660			
0.628	344.07	0.686			
0.690	343.90	0.716			
0.732	343.85	0.735			



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm³, ref. 3. Thorough mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Vötsch/Mel) (Cordoba Werke) and measured with a mercury manometer. High purity nitrogen was used for the backing pressure.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ±0.02 kg·m⁻³. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition < 0.002 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puris. p.a." material, purity >99.5 mass %; degassed ultrasonically, dried over molecular sieves 5A, no significant impurities by glc; $\rho(0, 298.15 \text{ K}) = 1.5264, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 786.79, T_{\text{b}}(0.0132 \text{ kPa/K}) = 337.42$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puris. p.a." material, purity >99 mass %; degassed ultrasonically, dried over molecular sieves 5A, no significant impurities by glc; $\rho(0, 298.15 \text{ K}) = 1.3208, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 894.27, T_{\text{b}}(0.0132 \text{ kPa/K}) = 350.13$.

Errors: |δT|/K = 0.02; |δP|/Pa = 200; |δx_i| = 0.003; |δy_i| = 0.02

REFERENCES

1. Int. DATA Ser., Ser. A, Guidelines 3b, 1994, 23(4).
2. Hisco, A. M.; Ortega, J. J. Chem. Eng. Data, 1998, 43, 618.
3. Ortega, J.; Peña, J.; de Alamos, C. J. Chem. Eng. Data, 1986, 37, 538.

Received: January 1, 2003

*Ser. A. Thermodynamic Properties of Non-reacting Binary Systems

Published: January 31, 2003

10/10/01-10/00001-1/0

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Int. DATA Ser., Ser. A, Guidelines 3b, 1994, 23(4)

SELECTED DATA ON MIXTURES

International Data Series*

No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

Components: 1. Methanol, CH₃O [67-56-1]
2. Ethyl ethanoate, C₄H₈O₂ [111-76-6]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature
x_i, mole fraction of component i in liquid phase
y_i, mole fraction of component i in vapor phase

Parameters: P, pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp}, data at variable x₁ and constant P, ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Duda, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-083 Warszawa, Poland)

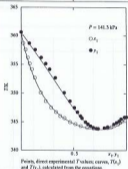
SOURCE OF DATA

Blanco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain). FIRST PUBLISHED RESULTS

Notes: The table opens smoothed values of T and calculated values of y₁

P/MPa = 141.3		
x ₁	T/K	y ₁
0.00	360.62	0.0000
0.05	356.74	0.1506
0.10	353.85	0.2589
0.15	351.63	0.3407
0.20	349.90	0.4051
0.25	348.53	0.4574
0.30	347.43	0.5001
0.40	345.83	0.5709
0.50	344.79	0.6287
0.60	344.15	0.6757
0.70	343.83	0.7241
0.75	343.78	0.7504
0.80	343.83	0.7798
0.85	344.01	0.8146
0.90	344.36	0.8500
0.95	345.01	0.9161
1.00	346.14	1.0000

Standard deviation σ(T), including standard deviation (10σ/95%), and absolute maximum deviation δ₁(T)/K at P/MPa = 141.3 are: exp.: 0.052, 0.030, 0.245.



Points, direct experimental T values; curves, T(x₁) and T(y₁), calculated from the equations.

EQUATIONS

$$G^E RT = -x_1 A_1 (x_1 + x_2) - x_2 A_2 (x_1 + x_2)$$

$$v_1 = \exp\left[-(A_1 + \frac{A_2^2}{RT})\right] \quad v_2 = \exp\left[-(A_2 + \frac{A_1^2}{RT})\right]$$

$$P = P_1^* y_1 + P_2^* y_2 = \sum_{i=1}^2 v_i P_i^* \exp\left[\frac{P_i^* - (P_i^* - P^*) - 2P_i^* (1 - y_i)^2}{RT}\right]$$

$$P_i^* = G^* - x_i (dG^*/dx_i)_{T,P} \quad A_i^* = G^* - x_i (dG^*/dx_i)_{T,P}$$

$B_1 A_{12} - B_{12} A_{11} + B_{22} B_1^2 C_1 = P_1^* P_2^*$ $P_1^* P_2^* = \exp[A_1 + B_1/(C_1 + 2TK)]$

COEFFICIENTS IN THE EQUATIONS

P/MPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
141.3	347.96 (15.7)	0 (0)	67.746 (9.3)	0 (0)

The standard deviations σ(a_i) of the coefficients a_i are given in parentheses.

P/MPa	a ₁	B ₁	C ₁	A ₂	B ₂	C ₂
141.3	18.18546	-3394.15	-44.02	14.12569	-3751.89	-60.68

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 141.3 MPa are reported in ref. 2.

Computations: The 27 T_{exp} data at 141.3 MPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies, g_i^E.

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients B_{ij}, ref. 5, and the molar volumes under saturation pressure V_i^S, ref. 6.

Errors: Standard deviation σ(T) = [2(T - T_{exp})²/(N + 2)]^{1/2}
Relative standard deviation 100σ(T)/T = 20[2(T - T_{exp})²/(N + 2)]^{1/2}
M, number of experimental points, ref. 2.
n, number of coefficients in the smoothing equation.

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- Ortega, J. *Int. DAT4 Ser., Ser. Data Minera. Ser. A*, 1983, 31, 14.
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SELECTED DATA ON MIXTURES

International DATA Series*

No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamic Research Center

Component:	1. Methanol, CH ₃ OH [507-56-1]
	2. Methyl bromide, CBr ₃ H [422-42-7]
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T, temperature x ₁ , mole fraction of component 1 in liquid phase y ₁ , mole fraction of component 1 in vapor phase
Parameters:	T, pressure
Method:	Direct measurement of T, x ₁ and y ₁ at constant P; ref. 1

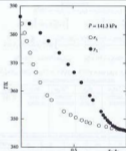
Author(s) of table:	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 36071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by:	Slawos, A.; Macyszek, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Blasen, A. M.; Ortega, J. Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain; ref. 2

DIRECT EXPERIMENTAL VALUES

P/P ₀ = 141.3						
x ₁	TK	y ₁	x ₁	TK	y ₁	
0.000	386.41	0.000	0.911	346.31	0.935	
0.005	383.94	0.086	0.935	346.39	0.947	
0.040	380.65	0.190	0.967	346.23	0.971	
0.060	377.83	0.266	0.983	346.13	0.984	
0.091	373.64	0.368	1.000	345.92	1.000	
0.120	369.63	0.450				
0.146	366.79	0.508				
0.186	363.19	0.576				
0.231	358.59	0.656				
0.290	356.90	0.685				
0.408	352.88	0.764				
0.470	351.53	0.782				
0.520	350.68	0.800				
0.577	349.67	0.823				
0.625	349.02	0.836				
0.655	348.64	0.849				
0.740	347.73	0.873				
0.813	347.50	0.894				
0.862	346.83	0.916				



Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebullimeter employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebullimeter was connected to a vacuum pump and a Fisher model VK1 pressure controller. High purity nitrogen was used for the backing pressure. The temperatures were measured by a ASL-F25 digital platinum resistance thermometer with a precision of readings ± 10 mK.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ± 0.02 kg m⁻³. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition < 0.002 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), degassed ultrasonically, dried over molecular sieves 3A.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity >99.0 mass %; degassed ultrasonically, dried over molecular sieves 3A;
 n_D^{20} , 298.15 K = 1.3812, ρ (298.15 K) kg m⁻³ = 492.26, T_c (0.132 MPa) K = 375.24

Errors: | δT | K = 0.01; | δP | Pa = 200; | δx_1 | = 0.002; | δy_1 | = 0.001.

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SELECTED DATA ON MIXTURES
International Data Series*
No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

Components: 1. Methanol, CH₃O (67-56-1)
2. Methyl Isocyanate, C₂H₃N (621-42-7)

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T, temperature
x_i, mole fraction of component i in liquid phase
y_i, mole fraction of component i in vapor phase

Parameters: P, pressure

Method: Calculations from direct experimental liquid-vapor equilibrium temperatures, T_{exp} data at variable x₁ and constant P, ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Czuga, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

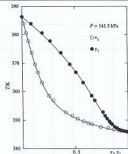
SOURCE OF DATA

Blasco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calculated values of y₁

P/Pa = 141.3		
x ₁	T/K	y ₁
0.00	386.41	0.0000
0.05	379.34	0.2230
0.10	372.31	0.3039
0.15	366.55	0.3163
0.20	362.07	0.3097
0.25	358.75	0.2956
0.30	356.28	0.2872
0.40	352.96	0.2710
0.50	350.89	0.2676
0.60	349.43	0.2618
0.70	348.29	0.2483
0.75	347.78	0.2650
0.80	347.31	0.2836
0.85	346.86	0.3051
0.90	346.49	0.3505
0.95	346.16	0.5614
1.00	345.97	1.0000

Standard deviation σ(T)/K, relative standard deviation 100σ(T)/T, and absolute maximum deviation Δ₁/173K at P/Pa = 141.3 are resp.: 0.125, 0.031, 0.182.



Points, direct experimental T values, T_{exp}(x₁) and T₁(y₁), calculated from the equations.

EQUATIONS

$$G^E/RT = -x_1^2(a_{12} + x_2^2b_{12}) - x_2^2(a_{21} + x_1^2c_{21})$$

$$v_1 = \exp\left[-(a_{11} + \frac{a_{12}^2}{2})/T\right] \quad v_2 = \exp\left[-(a_{22} + \frac{a_{21}^2}{2})/T\right]$$

$$P = P_1 + P_2 \sum_{i=1}^2 x_i^2 \exp\left[\frac{P_1^2 - (B_{12} - 17^2)(P - P_1^2) - 2P_2^2(1 - x_1)^2}{RT}\right]$$

$$P_1^2 = G^E - x_1^2(a_{12}^2 / 2a_{11}) \quad P_2^2 = G^E - x_2^2(a_{21}^2 / 2a_{22})$$

$$B_{12}^2 = B_{12} - (B_{11} + B_{22})/2, \gamma_1 = P_1/P; \quad P_1^2/\text{Pa} = \exp\{A_1 + B_1/C_1 + 20K\}$$

COEFFICIENTS IN THE EQUATIONS

P/Pa	a ₁₁ /K	a ₁₂ /K ²	a ₂₁ /K	a ₂₂ /K ²
141.3	3325.94 (2618.40)	-1284152 (661911)	-3355.82 (118.8)	1227289 (58267)

The standard deviations σ(a_{ij}) of the coefficients a_{ij} are given in parentheses.

P/Pa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
141.3	16.48187	-3567.82	-36.51	14.08347	-2926.32	-61.94

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 141.3 kPa are reported in ref. 2.

Computations: The 24 T_{exp} data at 141.3 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies g_i^E.

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_i were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid component with pressure were accounted for in terms of the 2nd virial coefficients B_{ii}, ref. 5, and the molar volumes under saturation pressure V_i^S, ref. 6.

Errors: Standard deviation σ(T) = [20(T - T_{exp})²(N - 2)]^{1/2}
Relative standard deviation 100σ(T)/T = 308[20(P - P_{exp})²/P_{exp}²(N - 2)]^{1/2}
N_i, number of experimental points, ref. 2
n_i, number of coefficients in the smoothing equation.

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- Ortega, J. *Int. Data Ser., Ser. A Data Mixtures*, Ser. A, 1980, 37, 96.
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- Thompson, C. *AIChE J.*, 1974, 20, 363, 1978, 21, 827.
- Yeo, L. C.; Woods, S. K. *AIChE J.*, 1966, 12, 95.

Compiled by Thermodynamics Research Center

Component:	1. Methanol, CH ₃ O [67-56-7] 2. Ethyl propanoate, C ₅ H ₁₀ O ₂ [105-35-1]
Status:	Binary system, single-phase liquid in equilibrium with vapor, pure components, both liquid in equilibrium with vapor
Variables:	T, temperature x _i , mole fraction of component i in liquid phase y _i , mole fraction of component i in vapor phase
Parameters:	P, pressure
Method:	Direct measurement of T, x _i , and y _i at constant P., ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Siroso, A.; Muznyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Bianco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/P ₀ = 101.3						
x ₂	T/K	y ₂	x ₁	T/K	y ₁	
0.080	383.24	0.008	0.750	347.54	0.851	
0.025	379.81	0.134	0.805	347.67	0.879	
0.052	375.09	0.257	0.861	346.70	0.906	
0.072	372.72	0.325	0.896	346.45	0.925	
0.086	370.90	0.375	0.926	346.20	0.941	
0.106	368.45	0.432	0.970	346.04	0.975	
0.125	366.49	0.476	0.985	346.00	0.985	
0.140	365.04	0.513	1.000	345.92	1.000	
0.170	362.67	0.561				
0.183	361.68	0.580				
0.206	360.22	0.606				
0.223	358.28	0.644				
0.260	357.21	0.662				
0.298	355.75	0.687				
0.349	353.83	0.720				
0.385	352.93	0.740				
0.441	351.40	0.767				
0.548	349.83	0.797				
0.664	348.46	0.828				

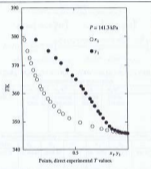
AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebullioscope employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm³, ref. 1. Turbulent mixing of the phases achieved equilibrium to be reached in a relatively short time. The ebullioscope was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Strossmüller Gesellschaften Werkheim) and measured with a mercury manometer. High purity nitrogen was used for the backing pressure.

Procedure: The procedure was described in ref. 1. The compositions were determined by measuring their densities at 298.15 K with an Astom Paar model DMA-35 vibrating-tube digital densimeter with a precision of ±0.02 kg m⁻³. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition = 0.002 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss. p.a." material, purity >99.5 mass %, degassed ultrasonically, dried over molecular sieves 3A; no significant impurities by glc, σD, 298.15 K = 1.3266, ρ(298.15 K)/kg m⁻³ = 788.79, T_b(101.32 kPa)/K = 337.42.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." material, purity >99 mass %, degassed ultrasonically, dried over molecular sieves 3A; no significant impurities by glc, σD, 298.15 K = 1.3815, ρ(298.15 K)/kg m⁻³ = 884.02, T_b(101.32 kPa)/K = 372.15.

Errors: ±0.7 K; ±0.01; ±0.01; ±0.01; ±0.01; ±0.01.



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2. Bianco, A. M.; Ortega, J. *J. Chem. Eng. Data*, 1998, 43, 635.
3. Ortega, J.; Pika, J. A.; de Abajo, C. *J. Chem. Eng. Data*, 1996, 41, 359.

SELECTED DATA ON MIXTURES

International Data Series*

No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

Components	1. Methanol, CH ₃ O (67-56-3) 2. Ethyl propanoate, C ₅ H ₁₀ O ₂ (103-37-3)
State	Binary system, single phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables	T, temperature x _i , mole fraction of component i in liquid phase y _i , mole fraction of component i in vapor phase
Parameters	P, pressure
Method	Calculation from direct experimental liquid-vapor equilibrium temperatures, T _{exp} , data at variable x ₁ and constant P, ref. 2.

Author(s) Ortega, I. Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, cf. table No. Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by Orosz, P. (Wydział Chemii, Uniwersytet Warszawski), ul. Pasteura 1, 02-093 Warszawa, Poland)

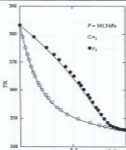
SOURCE OF DATA

Blanco, A. M.; Ortega, I. Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calculated values of y₁.

P/MPa = 141.3					
x ₁	T/K	y ₁			
0.00	343.29	0.0000			
0.05	375.47	0.2345			
0.10	368.18	0.3913			
0.15	364.30	0.5049			
0.20	360.68	0.5909			
0.25	357.78	0.6316			
0.30	355.60	0.6703			
0.40	352.57	0.7340			
0.50	350.57	0.7757			
0.60	349.14	0.8096			
0.70	348.85	0.8427			
0.75	347.56	0.8683			
0.80	347.15	0.8796			
0.85	346.75	0.9007			
0.90	346.38	0.9277			
0.95	346.20	0.9596			
1.00	345.92	1.0000			

Standard deviation, σ(T_{exp}), relative standard deviation 100σ(T_{exp})/T, and absolute maximum deviation Δ_{max}(T)/K at P/MPa = 141.3 are exp.: 0.092, 0.306, 0.171.



Points, direct experimental T values; curves, T(x₁, y₁) and T(y₁, x₁) calculated from the equations.

EQUATIONS

$$G^E/RT = -x_1b(x_1 + x_2y_2) - x_2b(x_2 + x_1y_1)$$

$$v_1 = \exp\left[-A_1 + \frac{B_1}{T}\right] \quad v_2 = \exp\left[-A_2 + \frac{B_2}{T}\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 v_i P_i^s \exp\left[\frac{P_i^s - (P_i^s - P_i^{s,0})^2 - 2P_i^{s,0}(1 - x_i)^2}{RT}\right]$$

$$P_i^s = G^s - x_i(10^6/RT)_{T,P} \quad P_i^{s,0} = G^s - x_i(10^6/RT)_{T,P}$$

$$R \ln \frac{P_i^s}{P_i^{s,0}} = (R_{i,1} - R_{i,2} + R_{i,3})/T; P_i^s/P_i^{s,0} = \exp\left[A_i + B_i/T + (R_{i,1} + R_{i,2} + R_{i,3})/T^2\right]$$

COEFFICIENTS IN THE EQUATIONS

P/MPa	A ₁ /K	A ₂ /K ²	B ₁ /K	B ₂ /K ²
141.3	4322.53	-1466204	-2468.68	784651
	(2895.6)	(885820)	(154.5)	(14360)

The standard deviations σ(A_i) of the coefficients A_i are given in parentheses.

P/MPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
141.3	16.48182	-3567.81	-36.51	14.14928	-2095.31	-44.15

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 141.3 kPa are reported in ref. 2.

Computations: The 27 T_{exp} data at 141.3 kPa were reduced using the modified Wilson equation, ref. 5, for the partial molar excess Gibbs energies g_i^E.

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameter A_i were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients B_i⁰, ref. 5, and the molar volumes under saturation pressure V_i⁰, ref. 6.

Errors: Standard deviation of T = [2(T_{exp} - T)²]/(N - 2)]^{1/2}
Relative standard deviation 100σ(T_{exp})/T = 100(T_{exp} - T)/T<sub>exp]^{1/2} = 2σ/T_{exp}^{1/2}
N, number of experimental points, ref. 2.
s, number of coefficients in the smoothing equation.</sub>

REFERENCES

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- Yeo, L. C.; Woods, S. S. *J. Res. Natl. Bur. Stand.*, 1966, 71, 95.

Compiled by Thermodynamic Research Center

Component(s):	1. Methanol, CH ₃ O [67-58-7] 2. Ethyl acetate, C ₄ H ₈ O ₂ [105-54-4]
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T, temperature x ₁ , mole fraction of component 1 in liquid phase y ₁ , mole fraction of component 1 in vapor phase
Parameters:	P, pressure
Method:	Direct measurement of T, x ₁ and y ₁ at constant P; ref. 1

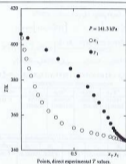
Author(s) of data:	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by:	Sikorski, A.; Majczyk, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Blasso, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/P ₀ = 141.3					
x ₁	TK	y ₁	x ₁	TK	y ₁
0.000	405.90	0.000	0.908	347.35	0.962
0.009	405.75	0.063	0.932	346.98	0.970
0.035	397.13	0.241	0.956	346.66	0.979
0.051	392.09	0.504	0.978	346.39	0.987
0.076	386.67	0.670	0.982	346.25	0.990
0.095	382.45	0.845	1.000	345.92	1.000
0.131	378.25	0.636			
0.162	371.75	0.692			
0.199	367.57	0.742			
0.260	362.65	0.799			
0.330	359.05	0.827			
0.386	355.75	0.855			
0.501	353.07	0.879			
0.578	351.75	0.891			
0.667	350.45	0.908			
0.724	349.75	0.919			
0.785	348.96	0.932			
0.849	348.13	0.946			
0.982	347.64	0.958			



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm³; ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a Vakumat electronic instrument (Nussloch/Gießhübel/Wertheim) and measured with a mercury manometer. High purity nitrogen was used for the backing process.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ±0.02 kg·m⁻³. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition < 0.002 mole fraction.

Materials: 1. Fluka AD (Buchs, St. Gallen, Switzerland), 'puris. p.a.' material, purity >99.5 mass-%; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; $\rho(298.15 \text{ K}) = 1.3386$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 786.79$, $T_f(101.32 \text{ kPa})/\text{K} = 337.42$.
2. Fluka AD (Buchs, St. Gallen, Switzerland), 'puris. p.a.' material, purity >98 mass-%; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; $\rho(298.15 \text{ K}) = 1.3098$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.54$, $T_f(101.32 \text{ kPa})/\text{K} = 294.18$.

Errors: |δT|/K = 0.01; |δP|/Pa = 200; |δx₁| = 0.003; |δy₁| = 0.01.

REFERENCES

1. In: *DATA Ser., Ser. A, Guidelines A*, 1994, 2(14).
2. Blasso, A. M.; Ortega, J. *J. Chem. Eng. Data*, 1998, 43, 636.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. *J. Chem. Eng. Data*, 1986, 31, 339.

SELECTED DATA ON MIXTURES
International Data Series*
No. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamic Research Center

National Institute of Standards and Technology, Boulder, CO 80505-3328

Components: 1. Methanol, CH₃O [67-56-1]
 2. Ethyl butanoate, C₆H₁₂O₂ [105-54-4]

State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor

Variables: T , temperature
 x_i , mole fraction of component i in liquid phase
 y_i , mole fraction of component i in vapor phase

Parameters: P , pressure

Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} , data at variable x_i and constant P , ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, de la Universidad de Las Palmas de Gran Canaria, 36071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Cray, T. (Wydział Chemii, Uniwersytet Warszawski, al. Politechniki 1, 02-093 Warszawa, Poland)

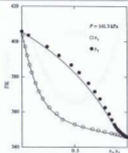
SOURCE OF DATA

Ortega, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); **FIRST PUBLISHED RESULTS**

Notes: The table reports smoothed values of T and calculated values of y_i .

P/Pa = 141.3							
x_1	T/K	y_1					
0.00	485.90	0.0000					
0.05	392.58	0.3128					
0.10	381.77	0.5125					
0.23	375.34	0.6356					
0.20	367.53	0.7124					
0.25	365.19	0.7825					
0.30	360.02	0.7965					
0.40	355.84	0.8406					
0.50	353.23	0.8892					
0.60	351.41	0.9313					
0.70	349.98	0.9616					
0.75	349.33	0.9225					
0.80	348.69	0.9336					
0.85	348.05	0.9466					
0.90	347.38	0.9614					
0.95	346.67	0.9791					
1.00	345.92	1.0000					

Standard deviation of T , $\sigma(T)$, relative standard deviation $100\sigma(T)/T$, and absolute maximum deviation $\Delta_{\text{max}}(T)/K$ at $P/Pa = 141.3$ are resp. 0.21, 0.757, 0.563.



Points, direct experimental T values; circles, $T(x_1)$ and $T(y_1)$, calculated from the equations.

EQUATIONS

$$G^E/RT = -a \ln(x_1 + c_1 x_1^2) - x_2^2(a_2 + c_2 x_2^2)$$

$$v_1 = \exp\left[-\ln(x_1 + \frac{a_1}{T})\right] \quad v_2 = \exp\left[-\ln(x_2 + \frac{a_2}{T})\right]$$

$$P = P_1 + P_2 + \sum_{j=1}^2 x_j^2 \exp\left[\frac{v_j^2 - (G_j - v_j^2)(P - P_j^s) - 2P_0^s(1 - v_j)^2}{RT}\right]$$

$$\mu_1^s = G^s - x_1^2(G^s/RT)_{x_1} \quad \mu_2^s = G^s - x_2^2(G^s/RT)_{x_2}$$

$B_{11}^E = B_{12}^E - (B_{11}^E + B_{22}^E)/2 - (v_1 - P_1)/P$; $P_j^s/Pa = \exp[A_j + B_j/(C_j + T/K)]$

P/Pa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
141.3	9218.32 (3258.4)	-3089569 (1159510)	-2286.43 (296.4)	812817 (120455)

The standard deviations $\sigma(a_i)$ of the coefficients a_i are given in parentheses.

P/Pa	A_1	B_1	C_1	A_2	B_2	C_2
141.3	36.48182	-3167.81	-36.51	12.38889	-2521.97	-112.77

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 141.3 kPa are reported in ref. 2.

Computations: The 25 T_{exp} data at 141.3 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies μ_i^E .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters A_{ij} were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd order virial coefficients B_{ij} , ref. 5, and the molar volumes under saturation pressure V_i^s , ref. 6.

Source: Standard deviation $\sigma(T) = [2(T - T_{\text{exp}})^2]/(N-2)^{1/2}$
 Relative standard deviation $100\sigma(T)/T = 100[2(T - T_{\text{exp}})^2]/(N-2)^{1/2}$
 N , number of experimental points, ref. 2
 n , number of coefficients in the smoothing equation.

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Composures:	1. Methanol, CH_3OH (67-56-1) 2. Ethyl ethanoate, $\text{C}_4\text{H}_8\text{O}_2$ (141-79-6)	Author(s):	Ortega, J. (Laboratorio de Termodinámica y Psicofísica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid; pure components, both liquid	Editor(s):	Strzeżek, A.; Mącznycki, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variable:	V^E , molar excess volume		
	x_i , mole fraction of component i		
Parameters:	T , temperature		
Constants:	P , pressure		
Method:	Calculation of V^E from density measurements at constant T and P and variable x_i , ref. 1		

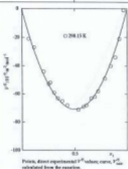
SOURCE OF DATA

1. Basso, A. M.; Ortega, J. (Laboratorio de Termodinámica y Psicofísica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: $P = 101.32 \text{ kPa}$

TK = 298.15			
x_1	$V^E_{100} / \text{m}^3 \cdot \text{mol}^{-1}$	x_1	$V^E_{100} / \text{m}^3 \cdot \text{mol}^{-1}$
0.9650	-21	0.9362	-21
0.1154	-27	0.9654	-1
0.2645	-44		
0.2321	-35		
0.2640	-52		
0.3099	-39		
0.3376	-63		
0.3794	-65		
0.4274	-68		
0.5327	-71		
0.5840	-68		
0.6077	-68		
0.6587	-63		
0.6985	-62		
0.7258	-54		
0.7855	-48		
0.8426	-48		
0.8867	-34		



SMOOTHING EQUATION

$$V^E_{\text{calc}} = x_1 x_2 \sum_{k=1}^6 a_k (x_1 - x_2)^{k-1}$$

Coefficients a_k in the smoothing equation, standard deviation σ_{fit} , and maximum deviation δ_{fit} determined by least-squares analysis.

TK	a_1	a_2	a_3	a_4	a_5	a_6	δ_{fit}
	$\text{m}^3 \cdot \text{mol}^{-1}$						
298.15	-282.6 (3.4)					2.9	8.4

The standard deviations σ_{a_i} of the coefficients a_i are given in parentheses. $\delta_{\text{fit}} = \max |V^E_{\text{calc}} - V^E|$; $\sigma_{\text{fit}} = [2(3^2 \sum_{i=1}^N (V^E_{\text{calc}} - V^E)^2) / (N-6)]^{1/2}$. N , number of direct experimental values; n , number of coefficients; a_i , all direct experimental values equally weighted.

AUXILIARY INFORMATION

Apparatus: The density was determined by an Anton Paar Model DMA-55 vibrating-tube digital densimeter with a precision of $\pm 0.02 \text{ kg} \cdot \text{m}^{-3}$. The temperature was controlled at $\pm 0.01 \text{ K}$ with a Heto-sterathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm³ glass vials. The apparatus was calibrated with doubly distilled and degassed water and benzene. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "pure, p.a." material, purity ≥ 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; $n_D(20, 298.15 \text{ K}) = 1.3296$, $d_{298.15 \text{ K}}(\text{kg} \cdot \text{m}^{-3}) = 786.79$, $V_m(181.32 \text{ kPa})/\text{K} = 357.42$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "pure, p.a." material, purity ≥ 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; no significant impurities by glc; $n_D(20, 298.15 \text{ K}) = 1.3700$, $d_{298.15 \text{ K}}(\text{kg} \cdot \text{m}^{-3}) = 894.27$, $V_m(181.32 \text{ kPa})/\text{K} = 350.13$.

Errors: $\delta TK = 0.02$; $\delta a_1 = 8.000$; $\delta V^E_{100} = 19 \text{ m}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$.

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- Ortega, J.; Basso, A. M.; Paz-Antón, M. L.; Andújar, E. *J. Chem. Thermodyn.*, 1995, 27, 1127.

SELECTED DATA FROM MIXTURES
International DATA Series*

No. EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80501-3328

Compiled by Thermodynamics Research Center

Components: 1. Methanol, CH₃O (67-58-7)
2. Ethyl propionate, C₅H₁₀O₂ (105-17-3)
State: Binary system, single-phase liquid, pure components, both liquid
Variables: V^E, molar excess volume
x₁, molar fraction of component 1
Parameters: T, temperature
Constants: P, pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x₁, ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 30071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Blasco, A.; Mayordoba, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

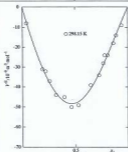
Blasco, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), ref. 2

INDIRECT EXPERIMENTAL VALUES

Notes: P = 101.32 kPa

TK = 298.15

x ₁	V ^E /10 ⁻⁶ m ³ mol ⁻¹								
0.0386	-8								
0.0887	-31								
0.2179	-32								
0.2557	-37								
0.3153	-44								
0.3956	-45								
0.4609	-58								
0.5284	-49								
0.6063	-39								
0.7261	-34								
0.7875	-28								
0.7991	-24								
0.8079	-24								
0.8627	-18								
0.8898	-14								
0.9415	-9								



Points, direct experimental V^E values; curve, V^E_{calc} calculated from the equation.

SMOOTHING EQUATION

$$V_{calc}^E = x_1 x_2 \sum_{i=1}^6 (v_i - x_j)^{i-1}$$

Coefficients v_i in the smoothing equation, standard deviation s_v, and maximum deviation s_m determined by least-squares analysis.

TK	v ₁	v ₂	v ₃	v ₄	v ₅	v ₆	s _v	s _m
	10 ⁻⁶ m ³ mol ⁻¹							
298.15	191.3 (3.4)	31.4 (3.3)	43.4 (24.4)				1.7	3.1

The standard deviations (s_v) of the coefficients v_i are given in parentheses. s_v = max{|v_{calc}^E - V^E|}; s_m = [Σ(v_{calc}^E - V^E)² / (N - 6)]^{1/2}. N, number of direct experimental values; v_i, number of coefficients v_i. All direct experimental values equally weighted.

AUXILIARY INFORMATION

Apparatus: The density was determined by an Anton Paar Model DMA-35 vibrating-tube digital densimeter with a precision of ±0.02 kg m⁻³. The temperature was controlled at ±0.01 K with a Deto ultrathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 25 cm³ glass vials. The apparatus was calibrated with doubly distilled and degassed water and ethanol. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss. p.a." material, purity >99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; w(1, 298.15 K) = 1.3266, ρ(298.15 K) kg m⁻³ = 786.79, T_g(101.32 kPa) K = 337.42.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." material, purity >99 mass %; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; w(1, 298.15 K) = 1.3015, ρ(298.15 K) kg m⁻³ = 882.02, T_g(101.32 kPa) K = 372.15.

Errors: ΔTK = 0.02, Δv_i = ±0.0005, ΔV^E/10⁻⁶ m³ mol⁻¹ < 2.

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- Ortega, J.; Mates, J. S.; Paz-Andrade, M. I.; Jimenez, E. *J. Chem. Thermodyn.*, 1993, 25, 1121.

Compiled by Thermodynamics Research Center

Component 1:	Methanol, CH ₃ O [67-58-1]
Component 2:	Ethyl acetate, C ₄ H ₈ O ₂ [101-14-1]
State:	Binary system, single-phase liquid, pure components, both liquid
Variables:	V^E , molar excess volume x_1 , mole fraction of component 1
Parameters:	T , temperature
Constants:	P , pressure
Method:	Calculation of V^E from density measurements at constant T and P and variable x_1 , ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 36071 Las Palmas de Gran Canaria, Canary Islands, Spain)

Edited by: Szwarc, A.; Marek, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

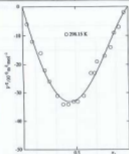
SOURCE OF DATA

Blazo, A. M.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: $P = 101.32 \text{ kPa}$

TK = 298.15	
x_1	$V^E/10^{-6} \text{ m}^3 \text{ mol}^{-1}$
0.0408	-6
0.0875	-12
0.2069	-22
0.3671	-34
0.5359	-36
0.7199	-34
0.8794	-24
0.9227	-14
0.9731	-3
0.9922	-3
0.9907	-3
0.9894	-3
0.9876	-3
0.9851	-3
0.9826	-3
0.9799	-3
0.9773	-3
0.9748	-3
0.9723	-3
0.9698	-3
0.9673	-3
0.9648	-3
0.9623	-3
0.9598	-3



Points, direct experimental V^E values; curve, V^E_{calc} calculated from the equation.

SMOOTHING EQUATION

$$V^E_{\text{calc}} = x_1 x_2 \sum_{i=1}^6 a_i (x_1 - x_2)^{i-1}$$

Coefficients a_i in the smoothing equation, standard deviation s_{calc} , and maximum deviation δ_{calc} determined by least-squares analysis.

TK	a_1	a_2	a_3	a_4	a_5	a_6	s_{calc}	δ_{calc}
	298.15	-129.3 (2.55)	47.8 (3.8)	47.1 (13.3)			1.8	3.4

The standard deviations s_{calc} of the coefficients a_i are given in parentheses
 $\delta_{\text{calc}} = \max |V^E_{\text{calc}} - V^E|$; $s_{\text{calc}} = [21]^{-1} \sum_{i=1}^N (V^E_{\text{calc}} - V^E)^2 / (N - 6)^{1/2}$
 N , number of direct experimental values; s_{calc} , number of coefficients- a_i
 All direct experimental values equally weighted

AUXILIARY INFORMATION

Apparatus: The density was determined by an Anton Paar Model DMA-15 vibrating-tube digital densimeter with a precision of $\pm 0.02 \text{ kg m}^{-3}$. The temperature was controlled at $\pm 0.01 \text{ K}$ with a Hele ultrathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm³ glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss. p.a." material, purity >99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A, no significant impurities by glc; $\rho(298.15 \text{ K}) = 1.5266$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 796.79$, $T_f(101.32 \text{ kPa})/\text{K} = 507.42$
 2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss. p.a." material, purity >99 mass %; degassed ultrasonically, dried over molecular sieves 3A; no significant impurities by glc; $\rho(298.15 \text{ K}) = 1.8996$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.54$, $T_f(101.32 \text{ kPa})/\text{K} = 394.18$.

Errors: ± 0.02 ; $\delta_{\text{calc}} = 0.0005$; $\delta V^E/10^{-6} \text{ m}^3 \text{ mol}^{-1} = 3$.

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