

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
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; ref. 1

Author(s) of table: Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)

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

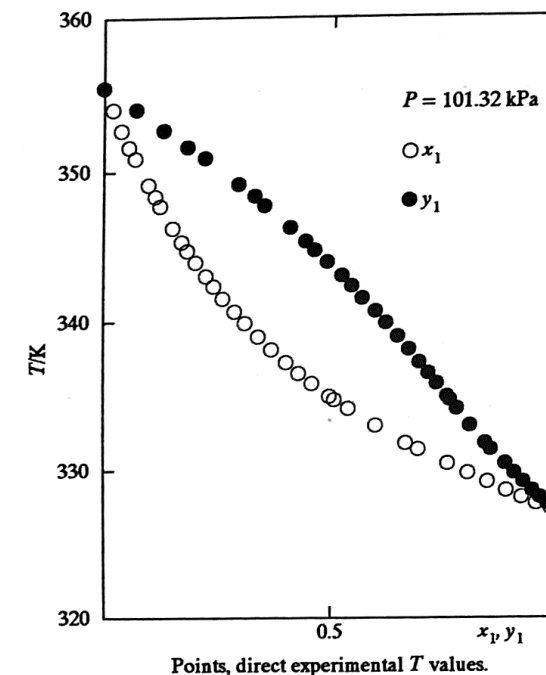
SOURCE OF DATA

Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32

x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	355.58	0.0000	0.4025	337.30	0.6939
0.0197	354.13	0.0712	0.4314	336.55	0.7143
0.0380	352.79	0.1306	0.4599	335.87	0.7318
0.0559	351.69	0.1837	0.4990	335.01	0.7555
0.0694	350.93	0.2210	0.5095	334.79	0.7611
0.0989	349.21	0.2961	0.5396	334.19	0.7770
0.1136	348.40	0.3303	0.5994	333.05	0.8066
0.1245	347.77	0.3530	0.6664	331.85	0.8393
0.1528	346.30	0.4097	0.6941	331.45	0.8525
0.1720	345.38	0.4427	0.7579	330.50	0.8842
0.1843	344.80	0.4626	0.8025	329.85	0.9044
0.2037	344.04	0.4907	0.8464	329.23	0.9246
0.2258	343.10	0.5224	0.8880	328.66	0.9443
0.2433	342.41	0.5452	0.9216	328.20	0.9611
0.2637	341.62	0.5679	0.9544	327.78	0.9773
0.2889	340.71	0.5964	0.9868	327.44	0.9933
0.3116	339.95	0.6194	1.0000	327.29	1.0000
0.3409	339.02	0.6460			
0.3704	338.18	0.6702			



AUXILIARY INFORMATION

Apparatus: The experimental equipment used to determine the isobaric VLE operated dynamically, with refluxing of both phases. System pressure was monitored by a model PPC2 pressure controller/calibrator from Desgranges et Hout, with an uncertainty of ±0.02 kPa. The temperature attained at each equilibrium stage was measured using a model ASL-F25 thermometer, calibrated periodically in accordance with the ITS-90, and had a measurement uncertainty of ±10 mK.

Procedure: The concentrations were calculated from the density curves as obtained using an Anton-Paar (DMA-55) densimeter with an uncertainty of ±0.02 kg m⁻³.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity 98 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3550, ρ(298.15 K)/kg·m⁻³ = 914.53.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity 99.7 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3820, ρ(303.15 K)/kg·m⁻³ = 775.37.

Errors: |δT|/K = 0.02; |δP|/Pa = 10; |δx₁| = 0.001; |δy₁| = 0.003.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).*
2. Ortega, J.; Espiau, F.; Postigo, M. *J. Chem. Eng. Data, 2003, 48, 916.*

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Int. DATA Ser., Sel. Data Mixtures, Ser. A 2005, 33(4), 289-296

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
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

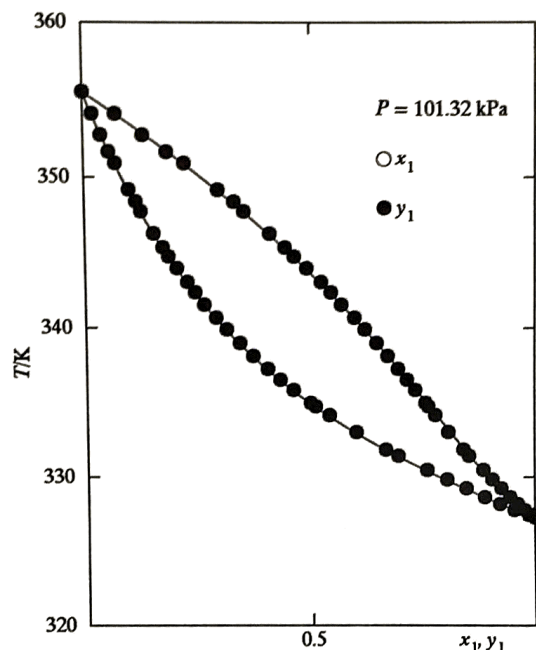
Author(s) Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

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Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-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/kPa = 101.32						
x ₁	T/K	y ₁				
0.00	355.58	0.0000				
0.05	352.11	0.1678				
0.10	349.09	0.2987				
0.15	346.46	0.4021				
0.20	344.15	0.4850				
0.25	342.13	0.5525				
0.30	340.35	0.6083				
0.40	337.36	0.6951				
0.50	334.98	0.7602				
0.60	333.02	0.8126				
0.70	331.35	0.8581				
0.75	330.59	0.8797				
0.80	329.88	0.9013				
0.85	329.19	0.9233				
0.90	328.54	0.9466				
0.95	327.90	0.9718				
1.00	327.29	1.0000				



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

EQUATIONS

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

$$c_1 = \exp\left[-(a_1 + \frac{a_2}{T})\right] \quad c_2 = \exp\left[-(a_3 + \frac{a_4}{T})\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp\left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1 - y_1)^2}{RT}\right]$$

$$\mu_1^E = G^E - x_2(\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1(\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; y_i = P_i/P; P_i^0/\text{kPa} = \exp[A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	225.75 (3.2)	0 (0)	14.771 (2.3)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.00356	-2535.15	-57.17	14.83933	-2658.29	-95.50

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.

Computations: The 36 T_{exp} data at 101.32 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 molar virial coefficients B_{ij}, ref. 5, and the molar volumes under saturation pressure V_i⁰, ref. 6.

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

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 289.
3. Wilson, G. M. J. Am. Chem. Soc., 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1969, k-5550, 1965, k-5030, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsonopoulos, C. AIChE J., 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J., 1966, 12, 95.

Compiled by Thermodynamics Research Center

Components: 1. Ethyl ethanoate, $C_4H_8O_2$ [141-78-6]
2. 2-Methyl-2-propanol, $C_4H_{10}O$ [75-65-0]
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 ; ref. 1

Author(s) of table: Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071 -Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Mączynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52,01 -224 Warszawa, Poland)

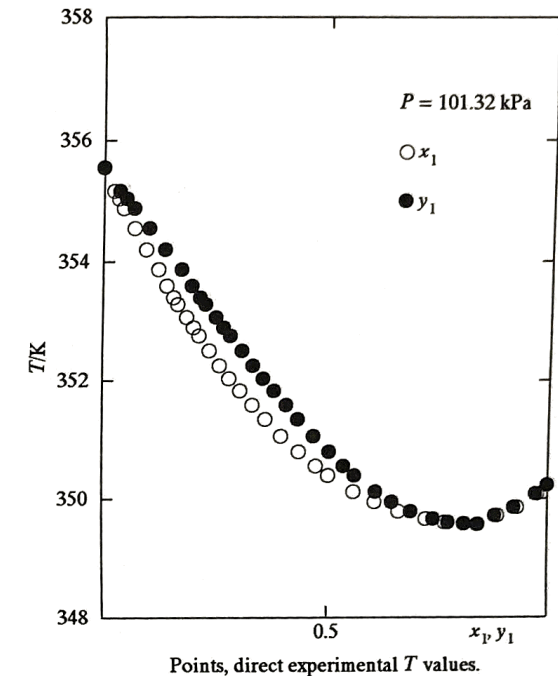
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Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071 -Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$

x_1	T/K	y_1	x_1	T/K	y_1
0.0000	355.58	0.0000	0.4025	337.30	0.6939
0.0234	355.18	0.0358	0.3991	351.08	0.4701
0.0334	355.06	0.0508	0.4386	350.81	0.5056
0.0447	354.90	0.0671	0.4771	350.58	0.5384
0.0686	354.57	0.1012	0.5052	350.41	0.5635
0.0947	354.21	0.1367	0.5619	350.14	0.6104
0.1235	353.88	0.1742	0.6098	349.97	0.6478
0.1417	353.61	0.1969	0.6629	349.81	0.6913
0.1573	353.41	0.2161	0.7244	349.68	0.7416
0.1668	353.30	0.2281	0.7679	349.63	0.7759
0.1857	353.08	0.2501	0.8102	349.60	0.8129
0.2009	352.91	0.2682	0.8428	349.59	0.8415
0.2139	352.77	0.2834	0.8878	349.74	0.8823
0.2369	352.52	0.3086	0.9322	349.88	0.9252
0.2599	352.27	0.3339	0.9778	350.10	0.9744
0.2823	352.05	0.3571	1.0000	350.25	1.0000
0.3063	351.84	0.3821			
0.3339	351.60	0.4091			
0.3625	351.36	0.4361			



AUXILIARY INFORMATION

Apparatus: The experimental equipment used to determine the isobaric VLE operated dynamically, with refluxing of both phases. System pressure was monitored by a model PPC2 pressure controller/calibrator from Desgranges et Hout, with an uncertainty of ± 0.02 kPa. The temperature attained at each equilibrium stage was measured using a model ASL-F25 thermometer, calibrated periodically in accordance with the ITS-90, and had a measurement uncertainty of ± 10 mK.
Procedure: The concentrations were calculated from the density curves as obtained using an Anton-Paar (DMA-55) densimeter with an uncertainty of ± 0.02 kg m⁻³.
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 303.15 \text{ K}) = 1.3675$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 894.44$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity 99.7 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 303.15 \text{ K}) = 1.3820$, $\rho(303.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 775.37$.
Errors: $|\delta T|/K = 0.02$; $|\delta P|/Pa = 10$; $|\delta x_1| = 0.001$; $|\delta y_1| = 0.003$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4)*.
2. Ortega, J.; Espiau, F.; Postigo, M. *J. Chem. Eng. Data, 2003, 48, 916*.

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Int. DATA Ser., Ser. A 2005, 33(4), 289-296

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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

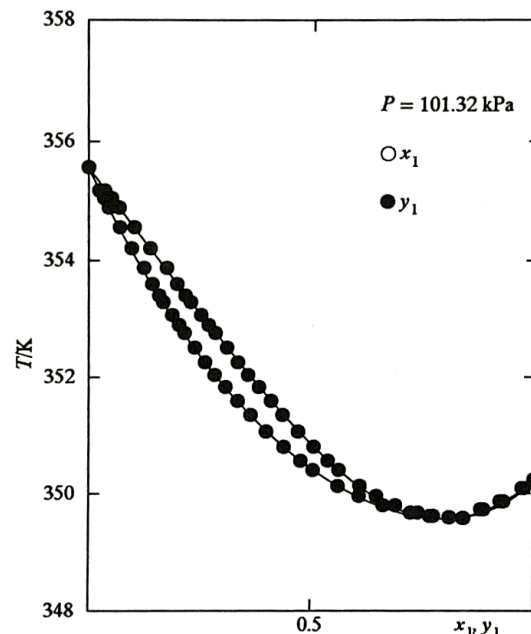
Author(s) Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-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/kPa = 101.32						
x ₁	T/K	y ₁				
0.00	355.58	0.0000				
0.05	354.82	0.0765				
0.10	354.13	0.1466				
0.15	353.49	0.2112				
0.20	352.91	0.2709				
0.25	352.38	0.3263				
0.30	351.91	0.3781				
0.40	351.10	0.4727				
0.50	350.46	0.5584				
0.60	350.00	0.6390				
0.70	349.70	0.7179				
0.75	349.62	0.7582				
0.80	349.60	0.7997				
0.85	349.63	0.8435				
0.90	349.74	0.8904				
0.95	349.93	0.9420				
1.00	350.25	1.0000				



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_2}{T} \right) / T \right] \quad c_2 = \exp \left[-\left(a_3 + \frac{a_4}{T} \right) / T \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^o \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^o)(P - P_i^o) - 2PB_{12}^E(1 - y_i)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22}) / 2; y_i = P_i / P; \quad P_i^o / \text{kPa} = \exp [A_i + B_i / (C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²	
101.32	185.65 (4.1)	0 (0)	-27.811 (2.9)	0 (0)	

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.12165	-2751.89	-60.68	14.83933	-2658.29	-95.50

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.

Computations: The 34 T_{exp} data at 101.32 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 molar virial coefficients B_{ij}, ref. 5, and the molar volumes under saturation pressure V_i^o, ref. 6.

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

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
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5. Tsonopoulos, C. AIChE J., 1974, 20, 263; 1975, 21, 827.
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Components: 1. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
 2. Ethyl propanoate, C₅H₁₀O₂ [105-37-3]
State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables: T, temperature
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Parameters: P, pressure
Method: Direct measurement of T, x_p, and y_l at constant P; ref. 1

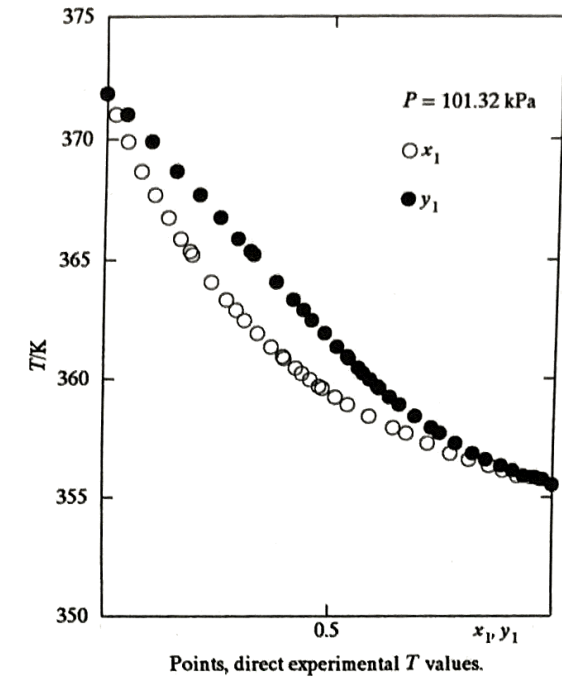
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DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32																			
x ₁	T/K	y ₁	x ₁	T/K	y ₁														
0.0000	371.91	0.0000	0.4579	360.01	0.5909														
0.0203	371.05	0.0448	0.4788	359.73	0.6074														
0.0478	369.94	0.1004	0.4859	359.64	0.6129														
0.0780	368.72	0.1556	0.5155	359.27	0.6355														
0.1090	367.73	0.2079	0.5435	358.94	0.6576														
0.1400	366.79	0.2544	0.5912	358.46	0.6918														
0.1684	365.91	0.2945	0.6448	357.99	0.7290														
0.1885	365.38	0.3210	0.6741	357.75	0.7483														
0.1944	365.24	0.3289	0.7209	357.31	0.7830														
0.2372	364.11	0.3800	0.7721	356.89	0.8214														
0.2715	363.36	0.4189	0.8135	356.63	0.8515														
0.2919	362.93	0.4408	0.8577	356.38	0.8853														
0.3115	362.51	0.4606	0.8898	356.19	0.9104														
0.3403	361.96	0.4888	0.9216	355.96	0.9359														
0.3711	361.39	0.5168	0.9542	355.88	0.9622														
0.3967	360.97	0.5396	0.9739	355.80	0.9782														
0.3995	360.91	0.5427	1.0000	355.58	1.0000														
0.4261	360.49	0.5643																	
0.4402	360.28	0.5761																	



AUXILIARY INFORMATION

Apparatus: The experimental equipment used to determine the isobaric VLE operated dynamically, with refluxing of both phases. System pressure was monitored by a model PPC2 pressure controller/calibrator from Desgranges et Hout, with an uncertainty of ±0.02 kPa. The temperature attained at each equilibrium stage was measured using a model ASL-F25 thermometer, calibrated periodically in accordance with the ITS-90, and had a measurement uncertainty of ±10 mK.
Procedure: The concentrations were calculated from the density curves as obtained using an Anton-Paar (DMA-55) densimeter with an uncertainty of ±0.02 kg m⁻³.
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity 99.7 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3820, ρ(303.15 K)/kg·m⁻³ = 775.37.
 2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3791, ρ(298.15 K)/kg·m⁻³ = 883.95.
Errors: |δT|/K = 0.02; |δP|/Pa = 10; |δx₁| = 0.001; |δy₁| = 0.003.

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1. *Int. DATA Ser., Ser. A, Guideline 3h*, 1994, 22(4).
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293 *Int. DATA Ser., Ser. A Data Mixtures, Ser. A 2005, 33(4), 289-296*

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Components: 1. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
2. Ethyl propanoate, C₅H₁₀O₂ [105-37-3]
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 temperature, T_{exp}, data at variable x_i and constant P; ref. 1

Author(s) Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)

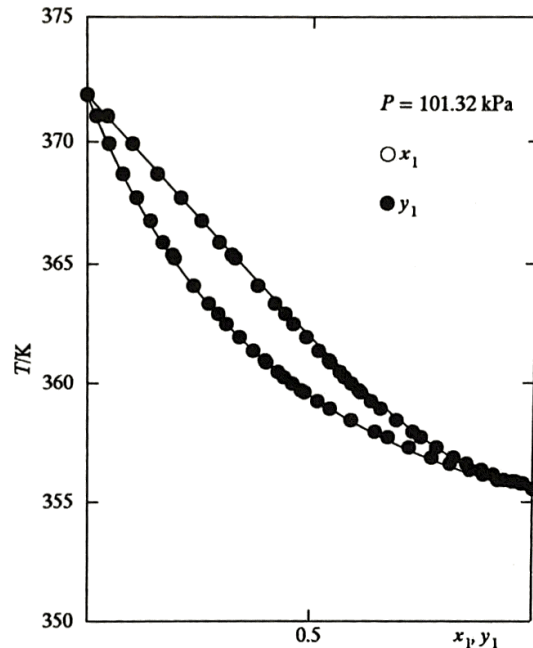
Edited by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-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/kPa = 101.32		
x ₁	T/K	y ₁
0.00	371.91	0.0000
0.05	369.78	0.1079
0.10	367.95	0.1988
0.15	366.38	0.2769
0.20	365.01	0.3450
0.25	363.81	0.4053
0.30	362.75	0.4594
0.40	360.97	0.5535
0.50	359.54	0.6348
0.60	358.37	0.7083
0.70	357.42	0.7778
0.75	357.01	0.8123
0.80	356.65	0.8470
0.85	356.32	0.8826
0.90	356.03	0.9195
0.95	355.78	0.9584
1.00	355.58	1.0000



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

EQUATIONS

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

$$c_1 = \exp\left[-\left(a_1 + \frac{a_2}{T}\right)/T\right] \quad c_2 = \exp\left[-\left(a_3 + \frac{a_4}{T}\right)/T\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^0 \exp\left[\frac{\mu_i^E - (B_{ii} - V_i^0)(P - P_i^0) - 2PB_{12}^E(1 - y_i)^2}{RT}\right]$$

$$\mu_1^E = G^E - x_2(\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1(\partial G^E / \partial x_1)_{T,P}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; y_i = P_i/P; P_i^0/\text{kPa} = \exp[A_i + B_i/(C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	148.03 (13.9)	0 (0)	-8.7999 (11.1)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.83933	-2658.29	-95.50	14.15529	-2935.11	-64.15

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.

Computations: The 36 T_{exp} data at 101.32 kPa were reduced using the modified Wilson μ_i^E 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 molar virial coefficients B_{ij}, ref. 5, and the molar volumes under saturation pressure V_i⁰, ref. 6.

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

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3m*, 1995, 23(2).
2. Ortega, J. *Int. DATA Ser., Sel. Data Mixtures, Ser. A*, 2003, 31, 293.
3. Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 127.
4. *TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons*, 1965, k-5030, 1996, k-5580, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsonopoulos, C. *AIChE J.*, 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. *AIChE J.*, 1966, 12, 95.

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Int. DATA Ser., Sel. Data Mixtures, Ser. A 2005, 33(4), 289-296

SELECTED DATA ON MIXTURES
International DATA Series*
3k LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

Components: 1. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
2. Ethyl butanoate, C₆H₁₂O₂ [105-54-4]
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 Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071 -Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Mączynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

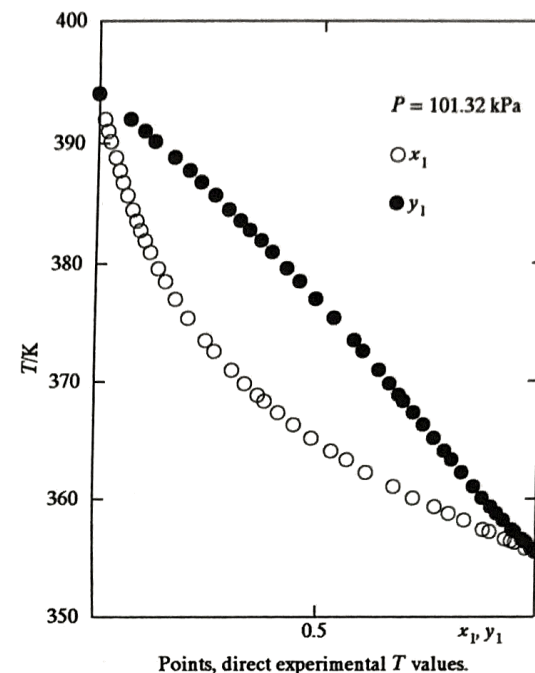
SOURCE OF DATA

Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071 -Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32

x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁							
0.0000	394.17	0.0000	0.3092	371.03	0.6368	0.9546	356.38	0.9796							
0.0145	392.07	0.0701	0.3381	369.93	0.6616	0.9782	355.90	0.9902							
0.0220	391.06	0.1025	0.3678	368.91	0.6835	1.0000	355.58	1.0000							
0.0280	390.22	0.1269	0.3831	368.42	0.6945										
0.0394	388.93	0.1705	0.4144	367.45	0.7165										
0.0490	387.84	0.2039	0.4497	366.42	0.7398										
0.0576	386.87	0.2315	0.4894	365.28	0.7648										
0.0680	385.74	0.2631	0.5339	364.21	0.7887										
0.0796	384.54	0.2942	0.5688	363.43	0.8061										
0.0895	383.63	0.3200	0.6129	362.37	0.8296										
0.0987	382.86	0.3421	0.6754	361.13	0.8569										
0.1099	381.96	0.3674	0.7203	360.20	0.8769										
0.1216	380.98	0.3918	0.7691	359.44	0.8968										
0.1400	379.66	0.4261	0.8017	358.85	0.9113										
0.1575	378.52	0.4559	0.8372	358.32	0.9265										
0.1805	377.06	0.4924	0.8799	357.49	0.9459										
0.2099	375.45	0.5334	0.8960	357.31	0.9530										
0.2486	373.55	0.5793	0.9310	356.71	0.9690										
0.2699	372.63	0.6007	0.9445	356.54	0.9750										



AUXILIARY INFORMATION

Apparatus: The experimental equipment used to determine the isobaric VLE operated dynamically, with refluxing of both phases. System pressure was monitored by a model PPC2 pressure controller/calibrator from Desgranges et Hout, with an uncertainty of ±0.02 kPa. The temperature attained at each equilibrium stage was measured using a model ASL-F25 thermometer, calibrated periodically in accordance with the ITS-90, and had a measurement uncertainty of ±10 mK.

Procedure: The concentrations were calculated from the density curves as obtained using an Anton-Paar (DMA-55) densimeter with an uncertainty of ±0.02 kg m⁻³.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity 99.7 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3820, ρ(303.15 K)/kg·m⁻³ = 775.37.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 98 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 303.15 K) = 1.3880, ρ(298.15 K)/kg·m⁻³ = 873.94.

Errors: |δT|/K = 0.02; |δP|/Pa = 10; |δx₁| = 0.001; |δy₁| = 0.003.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h*, 1994, 22(4).
2. Ortega, J.; Espiau, F.; Postigo, M. *J. Chem. Eng. Data*, 2003, 48, 916.

Components: 1. 2-Methyl-2-propanol, C₄H₁₀O [75-65-0]
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 x₁ and constant P; ref. 1

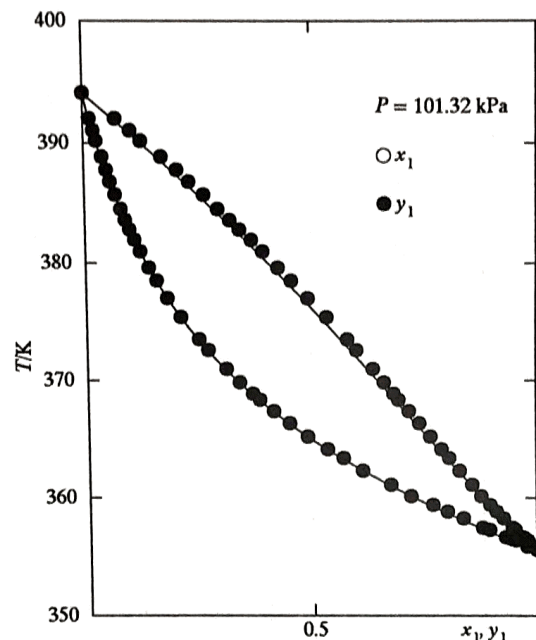
Author(s) Ortega, J. (Laboratorio Termodinámica y Físicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Orazc, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Espiau, F.; Postigo, M. (Laboratorio Termodinámica y Físicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-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/kPa = 101.32		
x ₁	T/K	y ₁
0.00	394.17	0.0000
0.05	387.60	0.1989
0.10	382.77	0.3334
0.15	379.02	0.4314
0.20	376.00	0.5069
0.25	373.50	0.5676
0.30	371.36	0.6180
0.40	367.87	0.6989
0.50	365.07	0.7634
0.60	362.72	0.8183
0.70	360.67	0.8675
0.75	359.72	0.8907
0.80	358.83	0.9132
0.85	357.97	0.9353
0.90	357.14	0.9570
0.95	356.35	0.9786
1.00	355.58	1.0000



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

EQUATIONS

$$P = \sum_{i=1}^2 x_i P_i^o \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^o)(P - P_i^o) - 2PB_{12}^E (1 - y_i)^2}{RT} \right]$$

$$y_i = \frac{x_i P_i^o}{P} \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^o)(P - P_i^o) - 2PB_{12}^E (1 - y_i)^2}{RT} \right]$$

$B_{12}^E = B_{12} - (B_{11} + B_{22})/2$; $P_i^o = P_{exp}(x_i = 1)$

The equations for μ_i^E are given in ref. 4.

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	-4.0146 (5.2)	0 (0)	149.33 (6.3)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.83933	-2658.29	-95.50	12.15904	-2121.97	-112.77

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.
Computations: The 41 T_{exp} data at 101.32 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 molar virial coefficients B_{ij}, ref. 5, and the molar volumes under saturation pressure V_i^o, ref. 6.
Errors: Standard deviation $\sigma(T) = [\sum (T - T_{exp})^2 / (N - n - 2)]^{1/2}$,
Relative standard deviation $100\sigma(\delta P/P) = 100[\sum ((P - P_{exp})/P_{exp})^2 / (N - n - 2)]^{1/2}$,
N, number of experimental points, ref. 2,
n, number of coefficients in the smoothing equation.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 295.
3. Wilson, G. M. J. Am. Chem. Soc., 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1965, k-5030, 1978, k-5620, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsonopoulos, C. AIChE J., 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J., 1966, 12, 95.