

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, $C_3H_6O_2$ [109-94-4]
2. Hexane, C_6H_{14} [110-54-3]
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: 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)

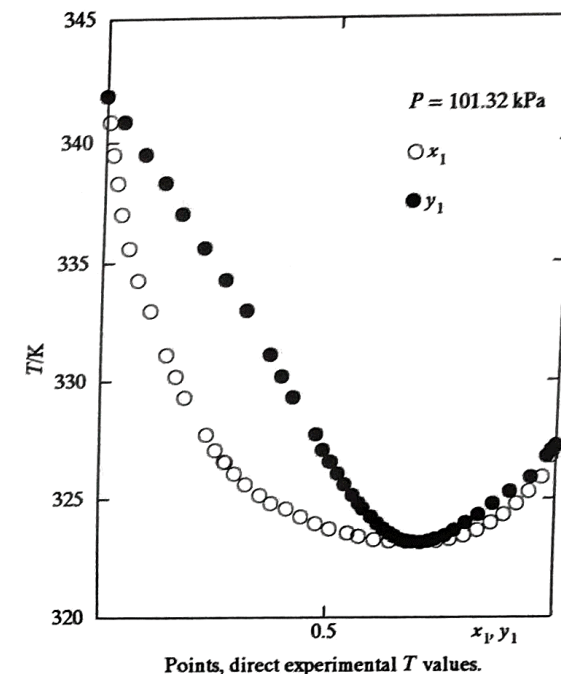
SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (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	341.93	0.0000	0.4134	324.62	0.5808	0.9904	326.84	0.9809
0.0073	340.89	0.0386	0.4466	324.28	0.6001	0.9955	327.08	0.9903
0.0173	339.55	0.0864	0.4780	324.01	0.6132	1.0000	327.29	1.0000
0.0281	338.35	0.1314	0.5099	323.79	0.6272			
0.0382	337.08	0.1692	0.5487	323.60	0.6405			
0.0574	335.65	0.2195	0.5740	323.47	0.6521			
0.0787	334.30	0.2692	0.6084	323.33	0.6655			
0.1082	333.02	0.3165	0.6420	323.25	0.6787			
0.1452	331.16	0.3709	0.6778	323.23	0.6926			
0.1654	330.23	0.3971	0.7092	323.21	0.7087			
0.1869	329.36	0.4229	0.7442	323.25	0.7255			
0.2355	327.77	0.4748	0.7744	323.34	0.7423			
0.2556	327.11	0.4909	0.8048	323.50	0.7626			
0.2757	326.64	0.5054	0.8345	323.71	0.7833			
0.2779	326.62	0.5089	0.8629	324.02	0.8077			
0.2991	326.11	0.5243	0.8900	324.38	0.8351			
0.3232	325.66	0.5407	0.9186	324.82	0.8654			
0.3556	325.21	0.5586	0.9442	325.35	0.9024			
0.3806	324.86	0.5716	0.9720	325.94	0.9473			



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 $\pm 0.02 \text{ kg m}^{-3}$.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3754$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 914.96$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3724$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 654.29$.

Errors: $|\delta T|/K = 0.03$; $|\delta P|/Pa = 50$; $|\delta x_1| = 0.003$; $|\delta y_1| = 0.005$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h*, 1994, 22(4).
2. Ortega, J.; Espiau, F.; Dieppa, R. *Fluid Phase Equilib.*, 2004, 215, 175.

0147-1503/5/04-297\$4.00

297

Int. DATA Ser., Sel. Data Mixtures, Ser. A 2005, 33(4), 297-306

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Hexane, C₆H₁₄ [110-54-3]
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)

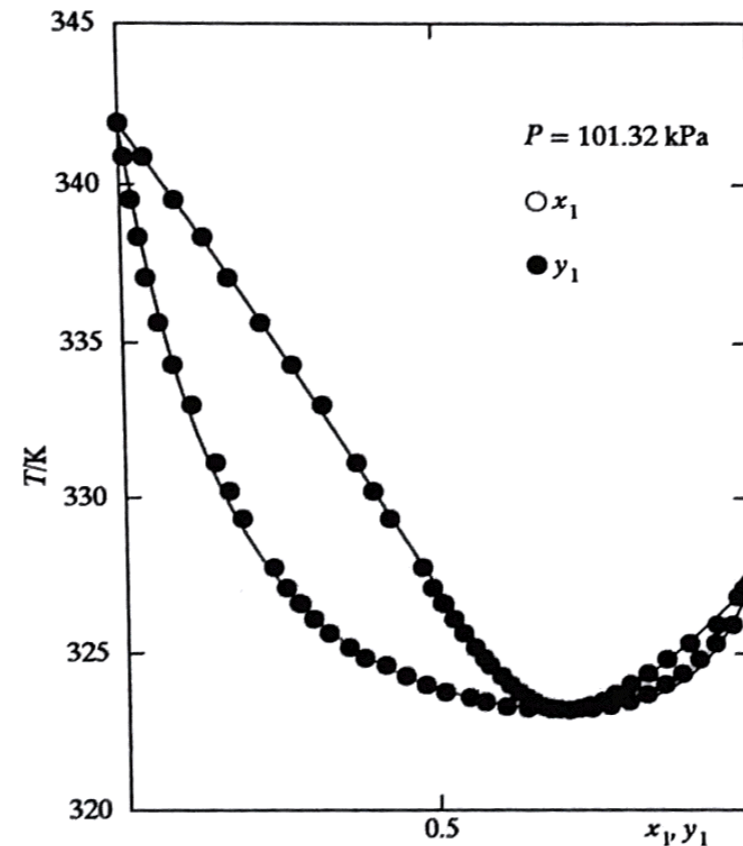
SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (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	341.93	0.0000
0.05	336.67	0.1886
0.10	333.07	0.3087
0.15	330.51	0.3911
0.20	328.64	0.4510
0.25	327.25	0.4966
0.30	326.20	0.5327
0.40	324.78	0.5875
0.50	323.93	0.6294
0.60	323.45	0.6665
0.70	323.27	0.7052
0.75	323.30	0.7277
0.80	323.45	0.7543
0.85	323.76	0.7878
0.90	324.35	0.8326
0.95	325.40	0.8974
1.00	327.29	1.0000

Standard deviation σ(T)/K, relative standard deviation 100σ(δP/P), and absolute maximum deviation δ_m(T)/K at P/kPa = 101.32 are resp.: 0.199, 0.662, 0.602.



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	341.48 (10.0)	0 (0)	175.12 (7.2)	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	14.78445	-3054.15	-26.87	13.81674	-2696.04	-48.83

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 refs 4 and 5 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. 6, and the molar volumes under saturation pressure V_i⁰, ref. 7.

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, 297.
3. Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 127.
4. *Floppy Book on Thermophysical Properties of Pure Substances*, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. *TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons*, 1994, k-1440, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
6. Tsonopoulos, C. *AIChE J.*, 1974, 20, 263; 1975, 21, 827.
7. Yen, L. C.; Woods, S. S. *AIChE J.*, 1966, 12, 95.

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

Compiled by Thermodynamics Research Center

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

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
 2. Heptane, C₇H₁₆ [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; 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: Mącznyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52,01 -224 Warszawa, Poland)

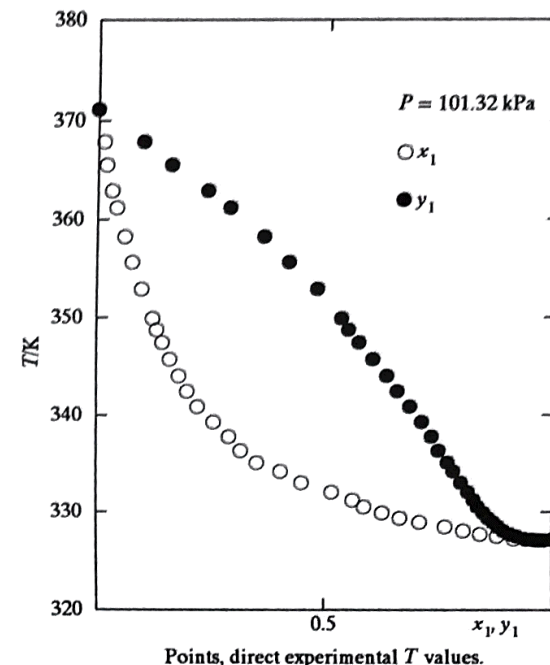
SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (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	371.18	0.0000	0.4070	334.26	0.7844
0.0140	368.00	0.0998	0.4532	333.13	0.8011
0.0203	365.65	0.1610	0.5206	332.14	0.8169
0.0330	363.03	0.2419	0.5668	331.32	0.8285
0.0436	361.30	0.2900	0.5904	330.67	0.8391
0.0621	358.40	0.3656	0.6300	330.05	0.8509
0.0789	355.80	0.4216	0.6695	329.48	0.8609
0.1005	353.01	0.4842	0.7119	329.03	0.8717
0.1246	350.00	0.5390	0.7682	328.56	0.8833
0.1341	348.85	0.5539	0.8075	328.19	0.8952
0.1459	347.55	0.5764	0.8444	327.86	0.9086
0.1636	345.80	0.6074	0.8809	327.59	0.9238
0.1835	344.08	0.6379	0.9182	327.36	0.9417
0.2020	342.54	0.6612	0.9446	327.25	0.9586
0.2246	340.96	0.6885	0.9669	327.21	0.9729
0.2605	339.39	0.7150	0.9838	327.19	0.9850
0.2934	337.85	0.7370	1.0000	327.29	1.0000
0.3202	336.42	0.7529			
0.3558	335.19	0.7720			



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 > 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3754, ρ(298.15 K)/kg·m⁻³ = 914.96
 2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3853, ρ(298.15 K)/kg·m⁻³ = 679.47.

Errors: |δT|/K = 0.03; |δP|/Pa = 50; |δx₁| = 0.003; |δy₁| = 0.005.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h*, 1994, 22(4).
2. Ortega, J.; Espiau, F.; Dieppa, R. *Fluid Phase Equilib.*, 2004, 215, 175.

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Heptane, C₇H₁₆ [142-82-5]
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: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

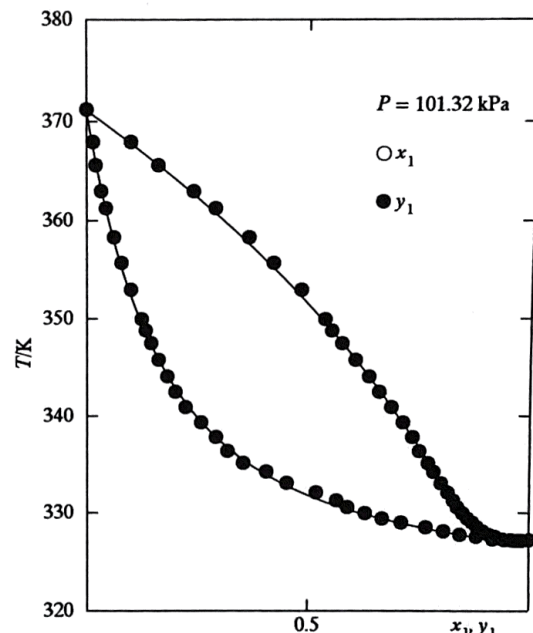
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FIRST PUBLISHED RESULTS

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	371.18	0.0000
0.05	360.07	0.3113
0.10	352.52	0.4821
0.15	347.13	0.5864
0.20	343.13	0.6555
0.25	340.07	0.7042
0.30	337.68	0.7402
0.40	334.26	0.7900
0.50	331.99	0.8236
0.60	330.40	0.8491
0.70	329.23	0.8716
0.75	328.74	0.8831
0.80	328.30	0.8957
0.85	327.90	0.9106
0.90	327.56	0.9298
0.95	327.31	0.9568
1.00	327.29	1.0000

Standard deviation σ(T)/K, relative standard deviation 100σ(δP/P), and absolute maximum deviation δ_m(T)/K at P/kPa = 101.32 are resp.: 0.266, 0.894, 0.481.



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	437.46 (13.5)	0 (0)	95.423 (6.5)	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	14.78445	-3054.15	-26.87	13.87301	-2910.26	-56.72

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 refs 4 and 5 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. 6, and the molar volumes under saturation pressure V_i^o, ref. 7.

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, 299.
3. Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 127.
4. *Floppy Book on Thermophysical Properties of Pure Substances*, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. *TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons*, 1991, k-1460, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
6. Tsionopoulos, C. *AIChE J.*, 1974, 20, 263; 1975, 21, 827.
7. Yen, L. C.; Woods, S. S. *AIChE J.*, 1966, 12, 95.

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, $C_3H_6O_2$ [109-94-4]
2. Octane, C_8H_{18} [111-65-9]
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: P , pressure
Method: Direct measurement of T , x_i and y_i at constant P ; ref. 1

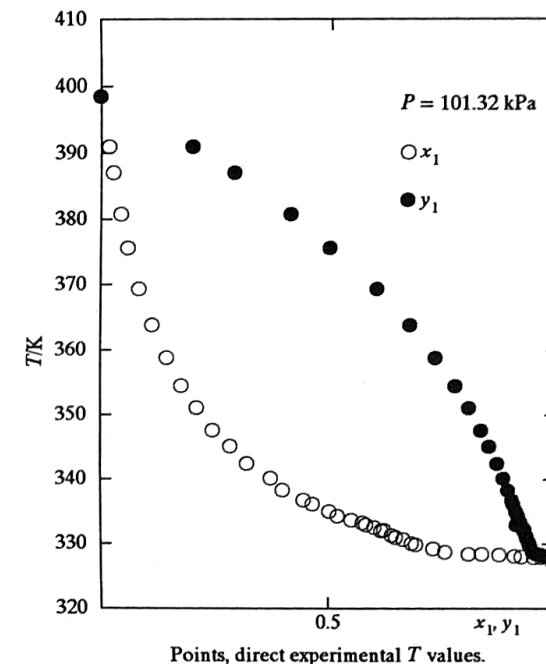
Author(s) of table: Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Mącztyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52,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

SOURCE OF DATA

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DIRECT EXPERIMENTAL VALUES

$P/\text{kPa} = 101.32$																	
x_1	T/K	y_1	x_1	T/K	y_1												
0.0000	398.65	0.0000	0.5537	333.82	0.9250	0.9752	328.03	0.9915									
0.0191	391.18	0.1986	0.5782	333.35	0.9276	1.0000	327.29	1.0000									
0.0281	387.25	0.2890	0.5862	333.09	0.9191												
0.0445	380.95	0.4123	0.6051	332.64	0.9324												
0.0604	375.80	0.4987	0.6199	332.11	0.9350												
0.0851	369.54	0.6027	0.6264	332.21	0.9365												
0.1138	363.94	0.6764	0.6424	331.43	0.9394												
0.1466	358.93	0.7342	0.6530	331.17	0.9411												
0.1788	354.60	0.7787	0.6692	330.79	0.9431												
0.2117	351.21	0.8085	0.6878	330.17	0.9470												
0.2474	347.67	0.8366	0.6965	330.03	0.9478												
0.2859	345.21	0.8554	0.7348	329.38	0.9524												
0.3227	342.51	0.8742	0.7615	328.89	0.9561												
0.3752	340.24	0.8883	0.8139	328.57	0.9638												
0.4023	338.46	0.8992	0.8433	328.54	0.9685												
0.4475	336.92	0.9075	0.8813	328.40	0.9749												
0.4675	336.22	0.9114	0.9154	328.27	0.9806												
0.5050	335.16	0.9173	0.9304	328.15	0.9832												
0.5228	334.37	0.9215	0.9590	328.06	0.9888												



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 > 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3754$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 914.96$
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3951$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 698.39$.
Errors: $|\delta T|/\text{K} = 0.03$; $|\delta P|/\text{Pa} = 50$; $|\delta x_1| = 0.003$; $|\delta y_1| = 0.005$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).*
2. Ortega, J.; Espiau, F.; Dieppa, R. *Fluid Phase Equilib., 2004, 215, 175.*

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Octane, C₈H₁₈ [111-65-9]
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: 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 Físicoquímica, 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)

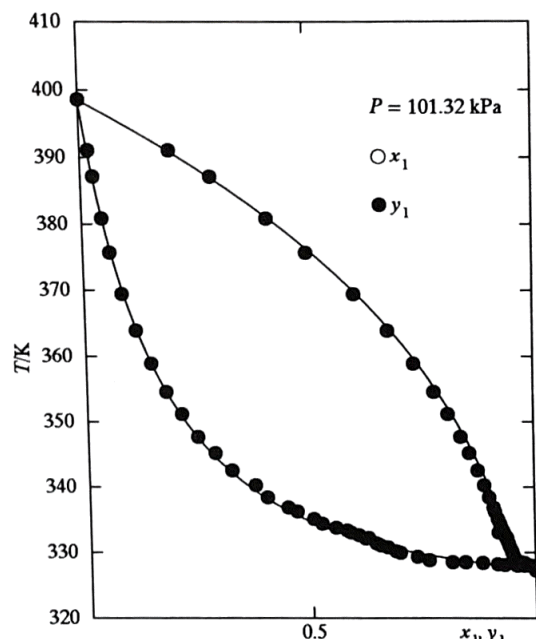
SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (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	398.66	0.0000				
0.05	379.57	0.4449				
0.10	367.20	0.6430				
0.15	358.63	0.7467				
0.20	352.35	0.8078				
0.25	347.57	0.8472				
0.30	343.84	0.8743				
0.40	338.44	0.9085				
0.50	334.83	0.9290				
0.60	332.36	0.9426				
0.70	330.64	0.9526				
0.75	329.98	0.9569				
0.80	329.40	0.9611				
0.85	328.88	0.9656				
0.90	328.38	0.9711				
0.95	327.85	0.9799				
1.00	327.29	1.0000				

Standard deviation σ(T)/K, relative standard deviation 100σ(δP/P), and absolute maximum deviation δ_m(T)/K at P/kPa = 101.32 are resp.: 0.415, 1.443, 0.821.



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	683.38 (23.9)	0 (0)	-3.3133 (6.8)	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	14.78445	-3054.15	-26.87	13.93730	-3123.13	-63.52

AUXILIARY INFORMATION

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

Computations: The 40 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 refs 4 and 5 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. 6, and the molar volumes under saturation pressure V_i⁰, ref. 7.

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, 301.
3. Wilson, G. M. J. Am. Chem. Soc., 1964, 86, 127.
4. Floppy Book on Thermophysical Properties of Pure Substances, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1990, k-1490, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
6. Tsonopoulos, C. AIChE J., 1974, 20, 263; 1975, 21, 827.
7. Yen, L. C.; Woods, S. S. AIChE J., 1966, 12, 95.

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, $C_3H_6O_2$ [109-94-4]
2. Nonane, C_9H_{20} [111-84-2]
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 Físicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Mącznyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

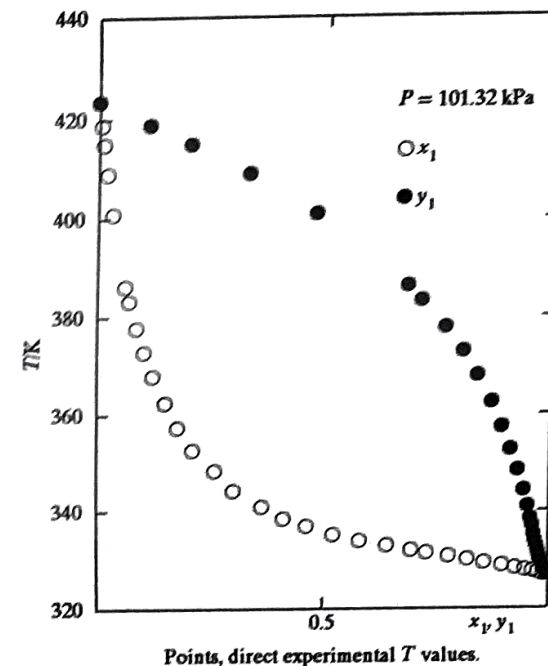
SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (Laboratorio Termodinámica y Físicoquímica, 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	423.66	0.0000	0.5832	334.08	0.9715
0.0058	419.03	0.1103	0.6438	333.20	0.9740
0.0111	415.15	0.2023	0.6970	332.26	0.9764
0.0194	409.20	0.3308	0.7314	331.70	0.9783
0.0328	401.08	0.4778	0.7807	330.95	0.9803
0.0623	386.50	0.6808	0.8209	330.34	0.9823
0.0706	383.50	0.7119	0.8585	329.64	0.9849
0.0871	377.90	0.7663	0.8980	329.07	0.9876
0.1050	372.95	0.8055	0.9274	328.54	0.9899
0.1245	368.05	0.8379	0.9492	328.13	0.9923
0.1528	362.60	0.8700	0.9667	327.77	0.9945
0.1804	357.43	0.8940	0.9777	327.51	0.9961
0.2135	352.87	0.9140	0.9898	327.17	0.9984
0.2637	348.62	0.9313	1.0000	327.29	1.0000
0.3053	344.46	0.9441			
0.3673	341.20	0.9538			
0.4154	338.70	0.9604			
0.4667	337.17	0.9645			
0.5243	335.44	0.9682			



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.
Procedures: 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 > 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n_D(298.15\text{ K}) = 1.3754$, $\rho(298.15\text{ K})/\text{kg m}^{-3} = 914.96$
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n_D(298.15\text{ K}) = 1.4030$, $\rho(298.15\text{ K})/\text{kg m}^{-3} = 713.85$.
Errors: $|\delta T|/K = 0.03$; $|\delta P|/Pa = 50$; $|\delta x_1| = 0.003$; $|\delta y_1| = 0.005$.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
2. Ortega, J.; Espiau, F.; Dieppa, R. *Fluid Phase Equilib.*, 2004, 215, 175.

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Nonane, C₉H₂₀ [111-84-2]
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)

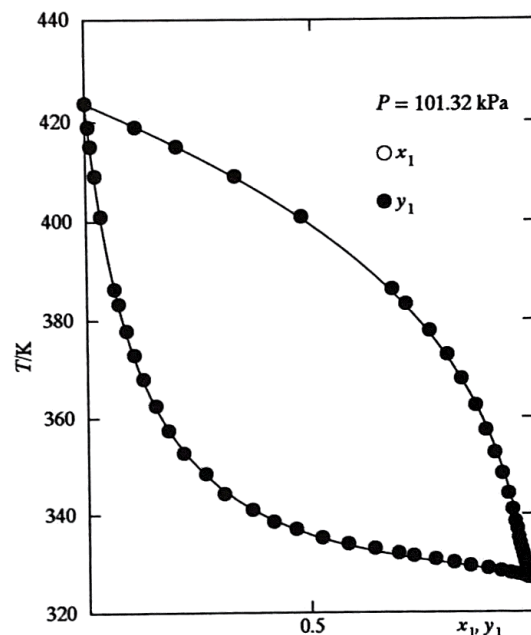
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FIRST PUBLISHED RESULTS

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	423.66	0.0000					
0.05	391.77	0.6109					
0.10	373.91	0.7955					
0.15	362.79	0.8704					
0.20	355.22	0.9082					
0.25	349.74	0.9300					
0.30	345.62	0.9440					
0.40	339.88	0.9604					
0.50	336.18	0.9695					
0.60	333.66	0.9754					
0.70	331.86	0.9798					
0.75	331.13	0.9817					
0.80	330.46	0.9836					
0.85	329.80	0.9857					
0.90	329.12	0.9884					
0.95	328.32	0.9924					
1.00	327.29	1.0000					

Standard deviation σ(T)/K, relative standard deviation 100σ(δP/P), and absolute maximum deviation δ_m(T)/K at P/kPa = 101.32 are resp.: 0.260, 0.945, 0.550.



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	598.55 (16.4)	0 (0)	40.739 (5.0)	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	14.78445	-3054.15	-26.87	13.99301	-3311.19	-70.46

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, 303.
3. Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 127.
4. *Floppy Book on Thermophysical Properties of Pure Substances*, 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.

AUXILIARY INFORMATION

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

Computations: The 33 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-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.

Compiled by Thermodynamics Research Center

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Decane, C₁₀H₂₂ [124-18-5]
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_p and y_l 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)

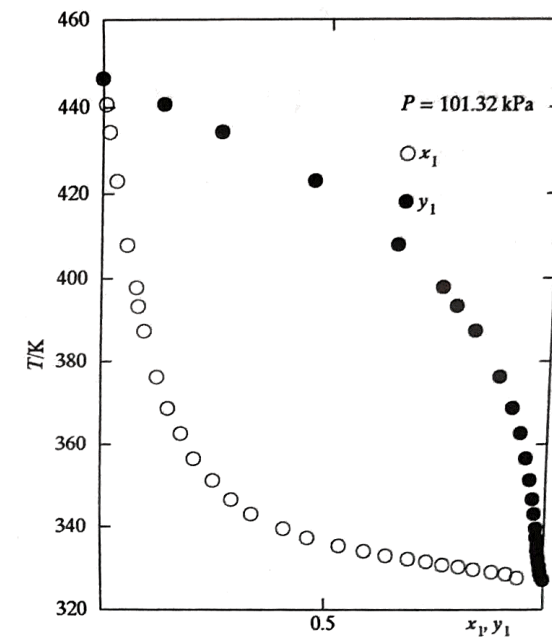
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Ortega, J.; Espiau, F.; Dieppa, R. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071 -Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32

x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	446.90	0.0000	0.6417	333.32	0.9880
0.0082	440.92	0.1345	0.6919	332.51	0.9890
0.0159	434.46	0.2606	0.7342	331.89	0.9899
0.0329	423.12	0.4649	0.7714	331.12	0.9910
0.0565	408.10	0.6523	0.8074	330.58	0.9919
0.0784	397.93	0.7549	0.8415	329.89	0.9926
0.0838	393.52	0.7876	0.8835	329.26	0.9935
0.0964	387.61	0.8303	0.9158	328.76	0.9944
0.1268	376.55	0.8889	0.9422	327.84	0.9963
0.1515	369.02	0.9199	1.0000	327.29	1.0000
0.1793	362.86	0.9393			
0.2096	356.87	0.9540			
0.2526	351.57	0.9647			
0.2940	346.91	0.9721			
0.3391	343.46	0.9769			
0.4100	339.87	0.9809			
0.4653	337.55	0.9837			
0.5356	335.73	0.9857			
0.5924	334.36	0.9869			



Points, direct experimental T values.

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 > 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15\text{ K}) = 1.3754$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 914.96$
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15\text{ K}) = 1.4095$, $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 726.19$.

Errors: $|\delta T|/\text{K} = 0.03$; $|\delta P|/\text{Pa} = 50$; $|\delta x_1| = 0.003$; $|\delta y_1| = 0.005$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3h*, 1994, 22(4).
2. Ortega, J.; Espiau, F.; Dieppa, R. *Fluid Phase Equilib.*, 2004, 215, 175.

0147-1503/5/504-305\$4.00

305

Int. DATA Ser., Sel. Data Mixtures, Ser. A 2005, 33(4), 297-306

Components: 1. Ethyl methanoate, C₃H₆O₂ [109-94-4]
2. Decane, C₁₀H₂₂ [124-18-5]
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

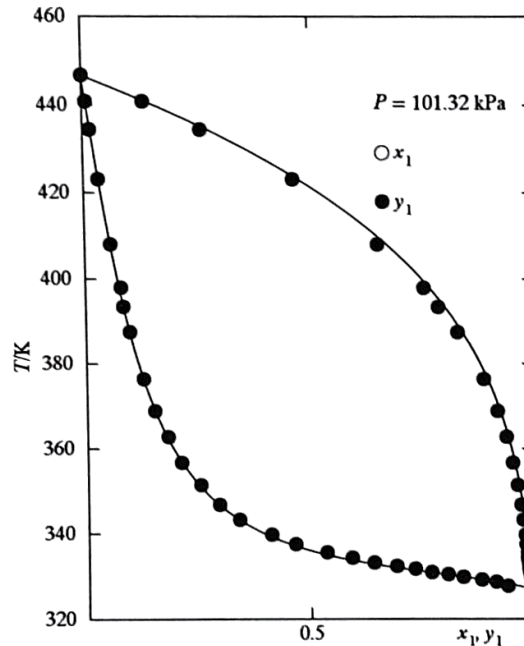
Author(s) Ortega, J. (Laboratorio Termodinámica y Fisicoquímica, Parque Científico-Tecnológico, Universidad de Las Palmas de Gran Canaria, 35071-Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by: Orazc, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Espiau, F.; Dieppa, R. (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	446.90	0.0000
0.05	412.22	0.6277
0.10	386.44	0.8489
0.15	369.74	0.9237
0.20	358.93	0.9536
0.25	351.66	0.9678
0.30	346.57	0.9756
0.40	340.13	0.9835
0.50	336.37	0.9874
0.60	333.98	0.9897
0.70	332.29	0.9913
0.75	331.57	0.9921
0.80	330.89	0.9929
0.85	330.19	0.9938
0.90	329.42	0.9950
0.95	328.50	0.9968
1.00	327.29	1.0000



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	536.94 (1118.4)	0 (0)	-1005.94 (35.9)	372701 (14597)

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	14.78445	-3054.15	-26.87	13.98359	-3442.76	-79.29

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.320 kPa are reported in ref. 2.

Computations: The 29 T_{exp} data at 101.320 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 refs 4 and 5 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. 6, and the molar volumes under saturation pressure V_i⁰, ref. 7.

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.

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