

Components: 1. Methyl ethanoate, $C_3H_6O_2$ [79-20-9]
2. 2-Propanol, C_3H_8O [67-63-6]

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_i , pressure

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

Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

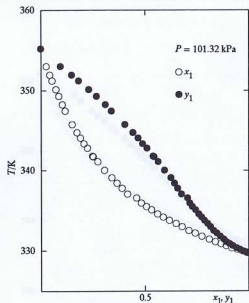
Edited by: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01 - 224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

$P/kPa = 74.66$						$P/kPa = 101.32$											
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1						
0.0000	347.65	0.0000	0.4903	327.30	0.7477	0.0000	355.26	0.0000	0.4836	336.03	0.7170						
0.0588	343.08	0.2170	0.5124	326.89	0.7558	0.0265	353.07	0.0957	0.5074	335.56	0.7290						
0.0742	342.02	0.2645	0.5436	326.34	0.7708	0.0432	351.98	0.1476	0.5318	335.16	0.7441						
0.0886	341.12	0.3022	0.5833	325.78	0.7886	0.0542	351.27	0.1811	0.5623	334.65	0.7602						
0.1064	339.95	0.3498	0.6174	325.28	0.8037	0.0717	350.18	0.2303	0.5892	334.27	0.7731						
0.1481	337.58	0.4312	0.6483	324.93	0.8168	0.0855	349.33	0.2675	0.6178	333.85	0.7874						
0.1863	335.79	0.4944	0.6846	324.45	0.8323	0.1038	348.32	0.3107	0.6505	333.43	0.8031						
0.2130	334.73	0.5291	0.7154	324.07	0.8460	0.1176	347.52	0.3407	0.6797	333.03	0.8173						
0.2290	334.08	0.5498	0.7328	323.85	0.8540	0.1503	345.84	0.4041	0.7124	332.57	0.8329						
0.2410	333.54	0.5635	0.7665	323.45	0.8692	0.1739	344.82	0.4426	0.7427	332.26	0.8480						
0.2620	332.87	0.5870	0.8028	323.03	0.8854	0.1904	344.16	0.4683	0.7759	331.86	0.8640						
0.2842	332.09	0.6088	0.8363	322.69	0.9015	0.2083	343.41	0.4899	0.8112	331.47	0.8808						
0.2977	331.77	0.6194	0.8643	322.40	0.9159	0.2248	342.86	0.5109	0.8406	331.18	0.8942						
0.3171	331.16	0.6372	0.8966	322.14	0.9333	0.2498	341.87	0.5401	0.8673	330.91	0.9095						
0.3329	330.72	0.6485	0.9302	321.79	0.9531	0.2529	341.77	0.5450	0.8926	330.67	0.9253						
0.3678	329.77	0.6753	0.9590	321.56	0.9712	0.2733	341.19	0.5648	0.9205	330.40	0.9426						
0.3967	329.16	0.6924	0.9808	321.40	0.9860	0.3056	340.09	0.5953	0.9455	330.19	0.9597						
0.4267	328.44	0.7102	1.0000	321.21	1.0000	0.3414	339.17	0.6256	0.9703	329.99	0.9776						
0.4561	327.90	0.7271				0.3656	338.50	0.6433	0.9893	329.87	0.9911						
						0.3913	337.87	0.6586	0.9923	329.79	0.9925						
						0.4168	337.13	0.6770	1.0000	329.76	1.0000						
						0.4605	336.64	0.7060									



Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ± 0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3593$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 926.99$.

2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3753$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 781.08$.

Errors: $|\delta T(\text{est.})|/K = 0.01$; $|\delta P(\text{est.})|/Pa = 20$; $|\delta x_1| = 0.001$ and 0.002 at 75 and 101 kPa; $|\delta y_1| = 0.005$ and 0.01 at 75 and 101 kPa.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1993, 26, 259.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

SELECTED DATA ON MIXTURES

International DATA Series*

3k. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. Methyl ethanoate, C₃H₆O₂ [79-20-9]
2. 2-Propanol, C₃H₈O [67-63-6]
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 de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

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

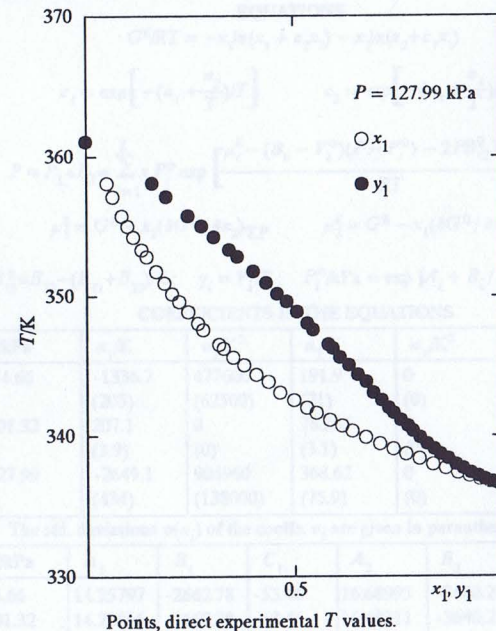
SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 127.99

x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	361.10	0.0000	0.4664	343.19	0.6906
0.0515	358.15	0.1596	0.5005	342.61	0.7104
0.0647	357.18	0.1937	0.5304	342.07	0.7280
0.0856	355.83	0.2455	0.5532	341.73	0.7397
0.0999	355.09	0.2779	0.5862	341.23	0.7572
0.1138	354.31	0.3071	0.6149	340.80	0.7735
0.1340	353.38	0.3446	0.6397	340.42	0.7860
0.1457	352.89	0.3642	0.6729	339.97	0.8030
0.1695	351.85	0.4029	0.7067	339.54	0.8201
0.1886	351.00	0.4337	0.7388	339.16	0.8365
0.2082	350.25	0.4604	0.7687	338.78	0.8528
0.2251	349.66	0.4837	0.8017	338.46	0.8700
0.2467	348.96	0.5083	0.8337	338.05	0.8889
0.2686	348.11	0.5317	0.8650	337.76	0.9063
0.2823	347.67	0.5454	0.8940	337.48	0.9251
0.3207	346.63	0.5833	0.9214	337.25	0.9426
0.3310	346.36	0.5933	0.9466	337.02	0.9592
0.3531	345.72	0.6113	0.9714	336.82	0.9774
0.3795	345.13	0.6322	0.9915	336.67	0.9926
0.4092	344.46	0.6531	1.0000	336.60	1.0000
0.4378	343.98	0.6732			



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerateban Wertheim) and measured with a mercury manometer. High purity nitrogen was used for the backing pressure.
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3593, ρ(298.15 K)/kg·m⁻³ = 926.99.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3753, ρ(298.15 K)/kg·m⁻³ = 781.08.
Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = 0.002; |δy₁| = 0.01.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).*
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1993, 26, 259.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

0147-1503/95/PS02-124\$2.20

©1995 Thermodynamics Research Center

124

Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995 23(2), 123-131

SELECTED DATA ON MIXTURES

International DATA Series*

3m. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. Methyl ethanoate, C₃H₆O₂ [79-20-9]
2. 2-Propanol, C₃H₈O [67-63-6]
State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables: T, temperature
y_i, mole fraction of component i in vapor phase
x_i, mole fraction of component i in liquid 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 Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., of table 3k: Canary Islands, Spain)
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

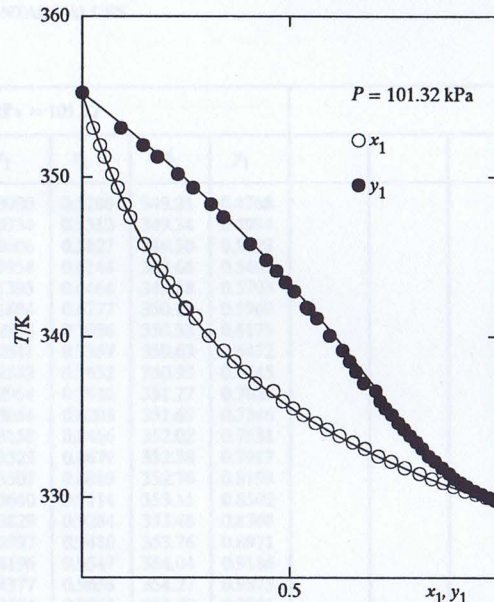
SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

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

x ₁	P/kPa = 74.66		P/kPa = 101.32		P/kPa = 127.99	
	T/K	y ₁	T/K	y ₁	T/K	y ₁
0.00	347.65	0	355.26	0	361.10	0
0.05	343.68	0.1930	351.58	0.1766	357.97	0.1534
0.10	340.34	0.3339	348.50	0.3083	355.15	0.2753
0.15	337.55	0.4381	345.91	0.4087	352.69	0.3713
0.20	335.22	0.5168	343.73	0.4871	350.57	0.4475
0.25	333.28	0.5777	341.87	0.5497	348.76	0.5089
0.30	331.65	0.6262	340.28	0.6008	347.20	0.5595
0.40	329.07	0.6993	337.70	0.6801	344.66	0.6396
0.50	327.11	0.7540	335.71	0.7403	342.66	0.7033
0.60	325.54	0.7997	334.11	0.7905	341.01	0.7592
0.70	324.22	0.8422	332.77	0.8363	339.61	0.8126
0.75	323.62	0.8637	332.17	0.8591	338.99	0.8398
0.80	323.07	0.8861	331.61	0.8826	338.41	0.8678
0.85	322.54	0.9100	331.09	0.9075	337.88	0.8972
0.90	322.05	0.9363	330.60	0.9346	337.40	0.9286
0.95	321.61	0.9659	330.15	0.9650	336.97	0.9627
1.00	321.21	1	329.76	1	336.60	1

Std. dev. σ(T)/K, rel. std. dev. 100σ(ΔP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 74.66 are resp.: 0.031, 0.127, 0.05.
at P/kPa = 101.32 are resp.: 0.054, 0.217, 0.177.
at P/kPa = 127.99 are resp.: 0.055, 0.21, 0.221.



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
74.66	-1336.7 (205)	477600 (62500)	191.9 (21)	0 (0)
101.32	207.1 (3.9)	0 (0)	76.335 (3.1)	0 (0)
127.99	-2649.1 (434)	904960 (138000)	368.62 (75.9)	0 (0)

The std. deviations σ(a_i) of the coeffs. a_i are given in parantheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
74.66	14.25797	-2662.78	-53.46	16.68995	-3640.2	-53.54
101.32	14.25556	-2662.78	-53.46	16.68311	-3640.2	-53.54
127.99	14.25642	-2662.78	-53.46	16.68769	-3640.2	-53.54

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 74.66, 101.32 and 127.99 kPa are reported in ref. 2.

Computations: The 37 T_{exp} data at 74.66 kPa, 43 T_{exp} data at 101.32 kPa and 41 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., 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 VLE data. 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 coeffs. B_{ij}; (ref. 5) and the molar volumes under saturation pressure V_i⁰ (ref. 6).

Errors: Std. dev. σ(T) = [Σ(T - T_{exp})² / (N - n - 2)]^{1/2},
Rel. std. dev. 100σ(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})² / (N - n - 2)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. 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 1995, 23, 123, 124.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1969, k-5550, 1965, k-5010, 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.

©1995 Thermodynamics Research Center

125

Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23(2), 123-131

SELECTED DATA ON MIXTURES

International DATA Series*

3k. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl propanoate, C₄H₈O₂ [554-12-1]
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 de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

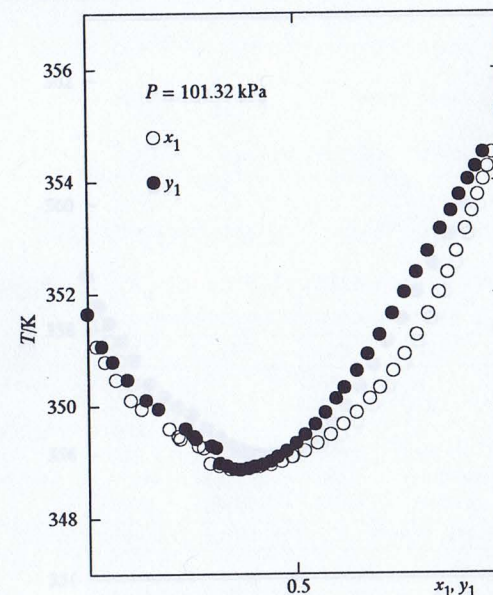
Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 74.66						P/kPa = 101.32					
x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	342.63	0.0000	0.4825	340.74	0.4347	0.0000	351.67	0.0000	0.5200	349.21	0.4768
0.0080	342.47	0.0138	0.5080	340.83	0.4511	0.0218	351.08	0.0334	0.5512	349.34	0.4994
0.0227	342.26	0.0354	0.5252	340.98	0.4669	0.0412	350.81	0.0606	0.5827	349.50	0.5223
0.0415	341.97	0.0625	0.5334	340.95	0.4687	0.0675	350.49	0.0954	0.6144	349.68	0.5463
0.0606	341.79	0.0868	0.5561	341.13	0.4877	0.1025	350.12	0.1395	0.6464	349.88	0.5703
0.0833	341.56	0.1146	0.5868	341.33	0.5094	0.1297	349.96	0.1694	0.6777	350.13	0.5969
0.1065	341.34	0.1425	0.6192	341.79	0.5327	0.1950	349.61	0.2338	0.7036	350.33	0.6175
0.1288	341.25	0.1648	0.6534	342.06	0.5586	0.2172	349.47	0.2541	0.7357	350.63	0.6472
0.1493	341.12	0.1870	0.6854	342.33	0.5841	0.2221	349.42	0.2582	0.7632	350.93	0.6745
0.1741	340.95	0.2106	0.7150	342.48	0.6086	0.2640	349.30	0.2954	0.7916	351.27	0.7027
0.2037	340.80	0.2373	0.7477	342.68	0.6379	0.2776	349.26	0.3064	0.8205	351.65	0.7346
0.2349	340.69	0.2631	0.7786	343.03	0.6689	0.2922	348.99	0.3158	0.8466	352.02	0.7631
0.2668	340.59	0.2888	0.8053	343.46	0.6973	0.3134	348.95	0.3323	0.8679	352.38	0.7917
0.2993	340.55	0.3142	0.8327	343.86	0.7275	0.3405	348.89	0.3507	0.8889	352.76	0.8198
0.3244	340.52	0.3328	0.8636	344.37	0.7671	0.3627	348.88	0.3660	0.9114	353.15	0.8502
0.3489	340.49	0.3470	0.8897	344.86	0.8027	0.3858	348.90	0.3829	0.9284	353.48	0.8768
0.3782	340.51	0.3668	0.9164	345.47	0.8428	0.4103	348.93	0.3997	0.9410	353.76	0.8971
0.4066	340.54	0.3850	0.9430	346.10	0.8880	0.4385	348.97	0.4196	0.9547	354.04	0.9186
0.4354	340.61	0.4037	0.9802	347.09	0.9592	0.4640	349.02	0.4377	0.9658	354.27	0.9373
0.4593	340.68	0.4190	1.0000	347.65	1.0000	0.4896	349.11	0.4554	0.9763	354.52	0.9561
						0.4910	349.11	0.4559	1.0000	355.26	1.0000



Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Gerateban Wertheim) and measured with a mercury manometer.
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3752, ρ(298.15 K)/kg·m⁻³ = 781.08.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3740, ρ(298.15 K)/kg·m⁻³ = 908.53.
Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = |δy₁| = 0.01 and 0.015 at 75 and 101 kPa.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).*
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1993, 26, 259.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

SELECTED DATA ON MIXTURES

International DATA Series*

3k. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl propanoate, C₄H₈O₂ [554-12-1]
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 de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

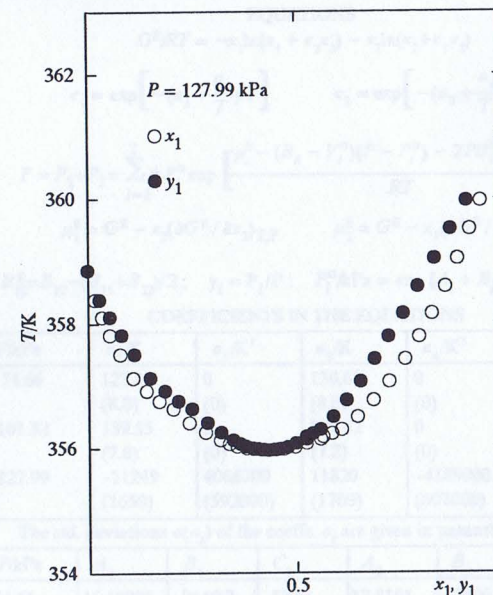
Edited by: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 127.99					
x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	358.87	0.0000	0.4709	356.00	0.4613
0.0165	358.40	0.0273	0.4966	356.03	0.4796
0.0337	358.12	0.0526	0.5252	356.09	0.5003
0.0526	357.83	0.0793	0.5582	356.15	0.5243
0.0770	357.52	0.1113	0.5648	356.19	0.5244
0.1075	357.14	0.1498	0.5858	356.24	0.5406
0.1395	356.93	0.1852	0.6097	356.31	0.5590
0.1701	356.77	0.2174	0.6475	356.51	0.5889
0.2040	356.65	0.2497	0.6869	356.78	0.6221
0.2437	356.42	0.2860	0.7247	357.08	0.6551
0.2817	356.27	0.3190	0.7624	357.44	0.6900
0.3162	356.14	0.3475	0.7967	357.80	0.7234
0.3382	356.08	0.3645	0.8279	358.17	0.7581
0.3571	356.04	0.3787	0.8599	358.60	0.7945
0.3796	356.01	0.3953	0.8895	359.06	0.8339
0.3962	356.00	0.4076	0.9189	359.53	0.8728
0.4148	355.99	0.4213	0.9439	359.98	0.9100
0.4313	355.98	0.4333	1.0000	361.10	1.0000
0.4509	355.99	0.4470			



Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Gerateban Wertheim) and measured with a mercury manometer. High purity nitrogen was used for the backing pressure.
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3752, ρ(298.15 K)/kg·m⁻³ = 781.08.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3740, ρ(298.15 K)/kg·m⁻³ = 908.53.
Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = 0.015; |δy₁| = 0.015.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1993, 26, 259.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

SELECTED DATA ON MIXTURES

International DATA Series*

3m. LIQUID-VAPOR EQUILIBRIUM

Published by Thermodynamics Research Center

The Texas A&M University System, College Station, TX 77843-3111

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl propanoate, C₄H₈O₂ [554-12-1]
State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables: T, temperature
y_i, mole fraction of component i in vapor phase
x_i, mole fraction of component i in liquid 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 Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., of table 3k; Canary Islands, Spain)
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

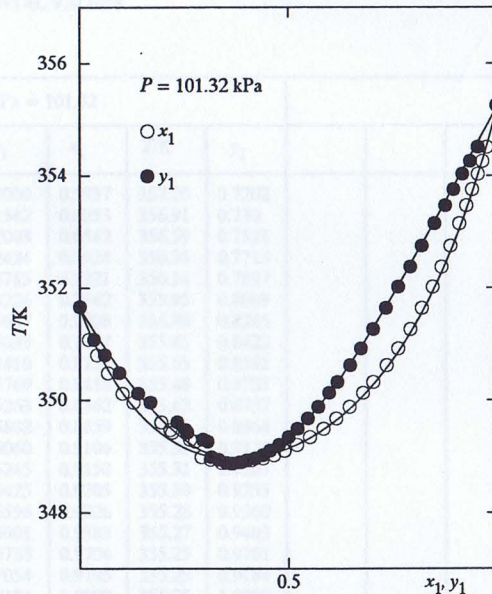
SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

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

x ₁	P/kPa = 74.66		P/kPa = 101.32		P/kPa = 127.99	
	T/K	y ₁	T/K	y ₁	T/K	y ₁
0.00	342.63	0	351.67	0	358.87	0
0.05	341.90	0.0714	350.82	0.0733	357.96	0.0738
0.10	341.38	0.1312	350.20	0.1353	357.33	0.1355
0.15	341.01	0.1827	349.73	0.1890	356.88	0.1897
0.20	340.77	0.2281	349.41	0.2365	356.55	0.2386
0.25	340.62	0.2690	349.18	0.2795	356.31	0.2837
0.30	340.55	0.3067	349.05	0.3190	356.15	0.3261
0.40	340.62	0.3763	348.99	0.3917	356.01	0.4047
0.50	340.91	0.4431	349.17	0.4607	356.07	0.4786
0.60	341.43	0.5128	349.60	0.5314	356.34	0.5517
0.70	342.23	0.5916	350.29	0.6099	356.87	0.6299
0.75	342.76	0.6368	350.77	0.6543	357.27	0.6736
0.80	343.41	0.6879	351.34	0.7040	357.79	0.7226
0.85	344.18	0.7468	352.05	0.7607	358.45	0.7788
0.90	345.12	0.8158	352.91	0.8266	359.24	0.8438
0.95	346.26	0.8986	353.97	0.9049	360.15	0.9182
1.00	347.65	1	355.26	1	361.10	1

Std. dev. σ(T)/K, rel. std. dev. 100σ(δP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 74.66 are resp.: 0.086, 0.342, 0.226.
at P/kPa = 101.32 are resp.: 0.081, 0.285, 0.18.
at P/kPa = 127.99 are resp.: 0.06, 0.202, 0.144.



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
74.66	123.4 (8.8)	0 (0)	130.62 (8.8)	0 (0)
101.32	139.55 (7.6)	0 (0)	109.62 (7.2)	0 (0)
127.99	-11249 (1650)	4066700 (592000)	11820 (1700)	-4189900 (607000)

The std. deviations σ(a_i) of the coeffs. a_i are given in parantheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
74.66	16.68995	-3640.2	-53.54	13.8151	-2600.93	-68.91
101.32	16.68311	-3640.2	-53.54	13.81665	-2600.93	-68.91
127.99	16.68769	-3640.2	-53.54	13.82191	-2600.93	-68.91

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 74.66, 101.32 and 127.99 kPa are reported in ref. 2.
Computations: The 40 T_{exp} data at 74.66 kPa, 42 T_{exp} data at 101.32 kPa and 37 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., 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 VLE data. 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 coeffs. B_{ij} (ref. 5) and the molar volumes under saturation pressure V_i⁰ (ref. 6).
Errors: Std. dev. σ(T) = [Σ(T - T_{exp})²/(N-n-2)]^{1/2},
Rel. std. dev. 100σ(δP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N-n-2)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. 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 1995, 23, 126, 127.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1965, k-5010, 1969, k-5580, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsoupoloulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

SELECTED DATA ON MIXTURES

International DATA Series*

3k. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl butanoate, C₅H₁₀O₂ [623-42-7]
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: Direct measurement of T, x_i, and y_i at constant P; ref. 1

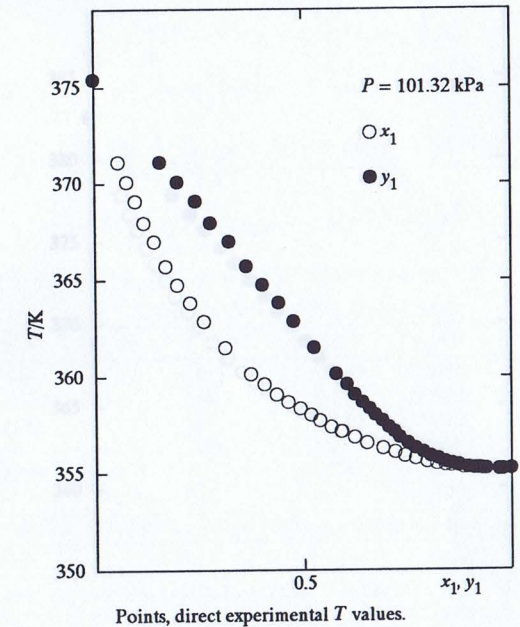
Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fiscoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)
Edited by: Mączynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01 -224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fiscoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 74.66						P/kPa = 101.32					
x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	365.07	0.0000	0.5831	348.98	0.6972	0.0000	375.46	0.0000	0.5937	357.20	0.7202
0.0670	360.90	0.1806	0.6068	348.81	0.7112	0.0591	371.16	0.1582	0.6253	356.91	0.730
0.0870	359.83	0.2237	0.6270	348.62	0.7224	0.0778	370.15	0.2003	0.6542	356.59	0.7521
0.1027	359.09	0.2552	0.6686	348.35	0.7448	0.0980	369.13	0.2424	0.6928	356.35	0.7713
0.1228	358.22	0.2913	0.7010	348.17	0.7628	0.1181	368.03	0.2785	0.7221	356.14	0.7897
0.1385	357.51	0.3181	0.7657	347.86	0.8027	0.1426	367.07	0.3226	0.7442	355.95	0.8069
0.1631	356.58	0.3551	0.8012	347.73	0.8265	0.1704	365.76	0.3647	0.7708	355.80	0.8246
0.1869	355.74	0.3887	0.8167	347.69	0.8353	0.1978	364.81	0.4033	0.7987	355.65	0.8422
0.2109	355.08	0.4201	0.8256	347.66	0.8433	0.2292	363.86	0.4410	0.8213	355.55	0.8581
0.2389	354.25	0.4515	0.8401	347.64	0.8521	0.2610	362.91	0.4769	0.8418	355.46	0.8735
0.2690	353.62	0.4806	0.8523	347.61	0.8628	0.3116	361.56	0.5263	0.8562	355.43	0.8737
0.3278	352.21	0.5314	0.8639	347.60	0.8701	0.3744	360.17	0.5802	0.8859	355.35	0.8964
0.3736	351.47	0.5667	0.8806	347.56	0.8845	0.4061	359.64	0.6060	0.9106	355.31	0.9176
0.4049	350.97	0.5909	0.8882	347.55	0.8894	0.4350	359.14	0.6245	0.9150	355.31	0.9207
0.4421	350.48	0.6133	0.9104	347.53	0.9080	0.4632	358.72	0.6425	0.9205	355.30	0.9255
0.4726	350.13	0.6320	0.9312	347.54	0.9263	0.4917	358.39	0.6596	0.9326	355.28	0.9360
0.4934	349.86	0.6472	0.9868	347.62	0.9838	0.5403	357.75	0.6901	0.9383	355.27	0.9403
0.5289	349.51	0.6666	0.9931	347.64	0.9909	0.5184	358.07	0.6735	0.9706	355.25	0.9701
0.5553	349.19	0.6810	1.0000	347.65	1.0000	0.5683	357.42	0.7054	0.9795	355.25	0.9784
						0.5917	357.20	0.7194	1.0000	355.26	1.0000



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm³, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakumat electronic instrument (Normschliff Gerateban Wertheim) and measured with a mercury manometer.
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3752, ρ(298.15 K)/kg·m⁻³ = 781.08.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3851, ρ(298.15 K)/kg·m⁻³ = 892.37.
Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = 0.001; |δy₁| = 0.002 and 0.005 at 75 and 101 kPa.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Susial, P. Ber. Bunsen-Ges. Phys. Chem. 1991, 95, 1214.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

0147-1503/95/9502-129\$2.20

©1995 Thermodynamics Research Center

129

Int. DATA Ser., Sel. Data Mixtures, Ser. A 1995, 23(2), 123-131

SELECTED DATA ON MIXTURES

International DATA Series*

3k. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl butanoate, C₅H₁₀O₂ [623-42-7]
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: Direct measurement of T, x_i, and y_i at constant P; ref. 1

Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

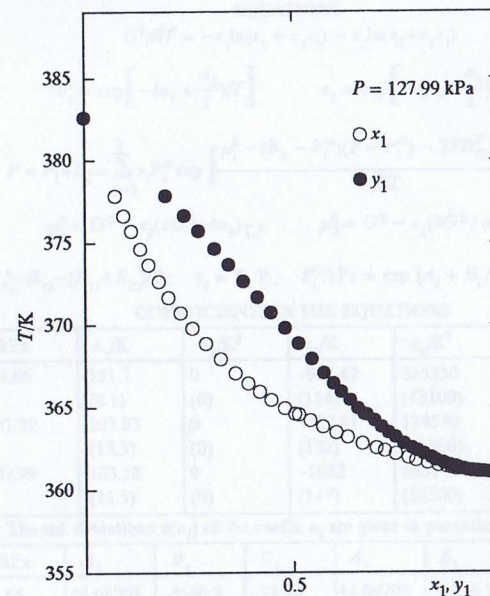
Edited by: Mączynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 127.99					
x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0000	382.67	0.0000	0.6318	363.24	0.7473
0.0734	377.90	0.1948	0.6682	362.87	0.7674
0.0943	376.71	0.2395	0.7022	362.58	0.7874
0.1125	375.77	0.2745	0.7215	362.43	0.7994
0.1344	374.70	0.3129	0.7471	362.22	0.8157
0.1542	373.73	0.3462	0.7782	362.01	0.8335
0.1790	372.70	0.3813	0.7970	361.86	0.8451
0.2023	371.74	0.4154	0.8253	361.69	0.8632
0.2306	370.81	0.4475	0.8500	361.55	0.8799
0.2591	369.87	0.4808	0.8700	361.44	0.8920
0.2914	368.93	0.5137	0.8816	361.37	0.9006
0.3267	367.98	0.5462	0.8934	361.32	0.9088
0.3620	367.13	0.5748	0.8970	361.30	0.9118
0.3928	366.50	0.5991	0.9214	361.22	0.9302
0.4195	366.00	0.6174	0.9306	361.20	0.9381
0.4470	365.52	0.6389	0.9402	361.17	0.9458
0.4796	365.01	0.6575	0.9468	361.15	0.9503
0.5048	364.65	0.6726	0.9575	361.13	0.9602
0.5145	364.62	0.6784	0.9725	361.11	0.9737
0.5421	364.26	0.6962	0.9818	361.09	0.9820
0.5721	363.88	0.7131	0.9889	361.08	0.9886
0.6046	363.53	0.7309	1.0000	361.10	1.0000



AUXILIARY INFORMATION

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

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.02 kPa, indicated by an electronic pressure gauge (MKS Baratron).

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3752, ρ(298.15 K)/kg·m⁻³ = 781.08.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); n(D, 298.15 K) = 1.3851, ρ(298.15 K)/kg·m⁻³ = 892.37.

Errors: |δT(estd.)|/K = 0.01; |δP(estd.)|/Pa = 20; |δx₁| = 0.002; |δy₁| = 0.007.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P. *Ber. Bunsen-Ges. Phys. Chem.* 1991, 95, 1214.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

SELECTED DATA ON MIXTURES

International DATA Series*

3m. LIQUID-VAPOR EQUILIBRIUM

The Texas A&M University System, College Station, TX 77843-3111

Published by Thermodynamics Research Center

Components: 1. 2-Propanol, C₃H₈O [67-63-6]
2. Methyl butanoate, C₅H₁₀O₂ [623-42-7]
State: Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables: T, temperature
y_i, mole fraction of component i in vapor phase
x_i, mole fraction of component i in liquid 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 Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., of table 3k: Canary Islands, Spain)

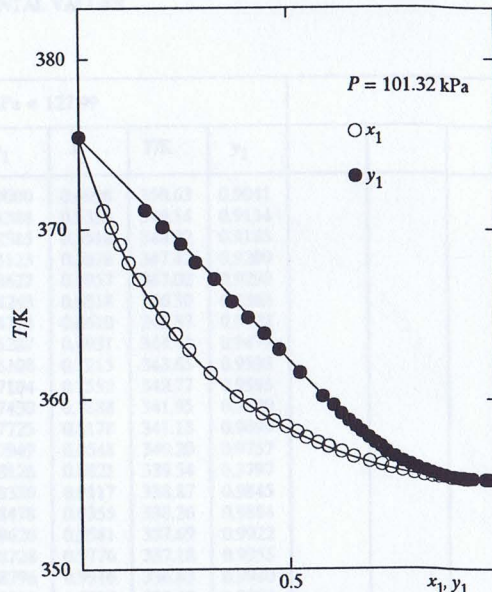
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); FIRST PUBLISHED RESULTS

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

x ₁	P/kPa = 74.66		P/kPa = 101.32		P/kPa = 127.99	
	T/K	y ₁	T/K	y ₁	T/K	y ₁
0.00	365.07	0	375.46	0	382.67	0
0.05	361.83	0.1421	371.87	0.1448	379.31	0.1343
0.10	359.21	0.2508	368.98	0.2552	376.40	0.2431
0.15	357.10	0.3358	366.65	0.3419	373.94	0.3312
0.20	355.38	0.4040	364.73	0.4119	371.87	0.4030
0.25	353.98	0.4599	363.15	0.4697	370.13	0.4624
0.30	352.82	0.5071	361.82	0.5187	368.68	0.5125
0.40	351.05	0.5841	359.76	0.5987	366.41	0.5939
0.50	349.78	0.6476	358.25	0.6640	364.76	0.6604
0.60	348.86	0.7055	357.13	0.7220	363.51	0.7203
0.70	348.19	0.7635	356.28	0.7784	362.55	0.7792
0.75	347.94	0.7942	355.95	0.8076	362.16	0.8097
0.80	347.74	0.8270	355.67	0.8385	361.83	0.8419
0.85	347.61	0.8628	355.46	0.8720	361.55	0.8762
0.90	347.54	0.9026	355.31	0.9090	361.34	0.9134
0.95	347.55	0.9478	355.23	0.9511	361.18	0.9544
1.00	347.65	1	355.26	1	361.10	1



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
74.66	151.7 (8.1)	0 (0)	-931.42 (114)	365350 (43100)
101.32	203.83 (13.3)	0 (0)	-432.91 (132)	174530 (51500)
127.99	103.18 (11.5)	0 (0)	-1682 (147)	663146 (58500)

The std. deviations σ(a_i) of the coeffs. a_i are given in parantheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
74.66	16.68995	-3640.2	-53.54	14.09705	-2926.72	-65.94
101.32	16.68311	-3640.2	-53.54	14.07396	-2926.72	-65.94
127.99	16.68769	-3640.2	-53.54	14.09238	-2926.72	-65.94

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 74.66, 101.32 and 127.99 kPa are reported in ref. 2.

Computations: The 38 T_{exp} data at 74.66 kPa, 40 T_{exp} data at 101.32 kPa and 44 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., 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 VLE data. 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 coeffs. B_{ij}; (ref. 5) and the molar volumes under saturation pressure V_i⁰ (ref. 6).

Errors: Std. dev. σ(T) = [Σ(T - T_{exp})²/(N - n - 2)]^{1/2},
Rel. std. dev. 100σ(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N - n - 2)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. 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 1995, 23, 129, 130.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1965, k-5010, 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.