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Components: 1. Methyl ethanoate, $C_3H_6O_2$ [79-20-9]
2. 1-Propanol, C_3H_8O [71-23-8]
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 Termodinámica y Fisicoquímica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

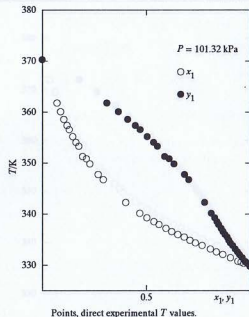
Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P.; de Alfonso, C. (Laboratorio de Termodinámica y Fisicoquímica, 35071 - University of Las Palmas de G. C., 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	370.35	0.0000	0.5367	338.60	0.8418
0.0705	361.85	0.3112	0.5623	338.05	0.8496
0.0870	360.15	0.3654	0.5956	337.25	0.8619
0.1026	358.65	0.4109	0.6231	336.65	0.8712
0.1191	357.45	0.4472	0.6528	336.10	0.8800
0.1292	356.65	0.4706	0.6827	335.55	0.8905
0.1462	355.25	0.5049	0.7111	334.95	0.8991
0.1618	354.15	0.5354	0.7373	334.45	0.9061
0.1755	353.35	0.5537	0.7694	333.95	0.9167
0.1946	351.35	0.5899	0.8086	333.25	0.9289
0.2123	350.95	0.6114	0.8390	332.65	0.9394
0.2288	349.95	0.6343	0.8693	332.15	0.9498
0.2699	347.85	0.6839	0.9061	331.55	0.9624
0.2934	346.85	0.7048	0.9412	330.85	0.9756
0.4022	342.35	0.7822	0.9573	330.65	0.9820
0.4685	340.25	0.8142	0.9711	330.40	0.9874
0.5035	339.35	0.8300	1.0000	329.82	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 Vakuumat electronic instrument (Normschiff 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.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "HPLC" grade material, degassed ultrasonically before use and stored in the dark for several days over molecular sieves; $n(D, 298.15\text{ K}) = 1.3593$, $\rho(298.15\text{ K})/\text{kg m}^{-3} = 926.99$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "purum" 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); $n(D, 298.15\text{ K}) = 1.3835$, $\rho(298.15\text{ K})/\text{kg m}^{-3} = 799.65$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/kPa = 20$; $|\delta x_1| = 0.003$; $|\delta y_1| = 0.01$.

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Ortega, J.; Susial P.; de Alfonso, C. *J. Chem. Eng. Data* 1990, 35, 350.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

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Components: 1. Methyl ethanoate, C₂H₆O₂ [79-20-9]
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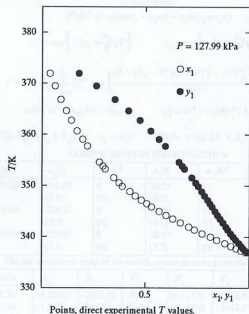
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SOURCE OF DATA

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 = 114.66						P/kPa = 127.99											
x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁						
0.0108	371.85	0.0627	0.6276	340.39	0.8648	0.0389	372.01	0.1781	0.5077	346.54	0.8125						
0.0452	368.13	0.2102	0.6528	339.77	0.8762	0.0633	369.60	0.2638	0.5312	345.93	0.8225						
0.0955	363.24	0.3746	0.6834	339.05	0.8872	0.0904	366.94	0.3523	0.5670	345.06	0.8368						
0.1172	361.25	0.4320	0.7175	338.34	0.8986	0.1175	364.73	0.4181	0.6015	344.30	0.8493						
0.1294	360.49	0.4557	0.7678	337.57	0.9122	0.1415	362.82	0.4741	0.6337	343.59	0.8620						
0.1650	357.74	0.5287	0.7975	337.03	0.9213	0.1698	360.79	0.5260	0.6709	342.83	0.8754						
0.2023	355.27	0.5870	0.8066	336.80	0.9252	0.1963	359.13	0.5658	0.7114	341.99	0.8897						
0.2159	354.53	0.6048	0.8231	336.47	0.9318	0.2198	357.81	0.5976	0.7381	341.46	0.8990						
0.2433	352.90	0.6396	0.8465	336.11	0.9388	0.2788	354.65	0.6629	0.7752	340.72	0.9119						
0.3177	349.34	0.7122	0.8616	335.95	0.9435	0.2950	353.90	0.6785	0.8149	340.07	0.9244						
0.3464	348.19	0.7333	0.8877	335.38	0.9537	0.3069	353.36	0.6900	0.8466	339.44	0.9374						
0.4055	346.20	0.7702	0.9065	335.12	0.9604	0.3484	351.63	0.7250	0.8846	338.78	0.9516						
0.4253	345.56	0.7827	0.9204	334.80	0.9663	0.3738	350.64	0.7426	0.9145	338.25	0.9630						
0.4714	344.24	0.8036	0.9409	334.42	0.9744	0.3888	349.92	0.7548	0.9388	337.81	0.9728						
0.4973	343.50	0.8151	0.9584	334.13	0.9815	0.4258	348.92	0.7730	0.9619	337.39	0.9825						
0.5328	342.58	0.8296	0.9732	333.88	0.9877	0.4524	348.09	0.7864	0.9840	337.03	0.9922						
0.5609	341.87	0.8413	0.9852	333.69	0.9931	0.4818	347.23	0.8010									
0.5930	341.17	0.8527															



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 Geratoben 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), "purum" grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves; n(D, 298.15 K) = 1.3593, ρ(298.15 K)/kg·m⁻³ = 926.99.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puris 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) = 1.3835, ρ(298.15 K)/kg·m⁻³ = 799.65.

Errors: |δT(est.)|/K = 0.01; |δP(est.)|/Pa = 20; |δx₁| = 0.003; |δy₁| = 0.01.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1990, 23, 621.
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. Methyl ethanoate, C₃H₆O₂ [79-20-9]
2. 1-Propanol, C₃H₈O [71-23-8]
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 x₂ and constant P; ref. 1

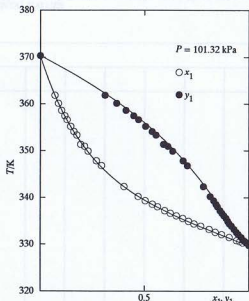
Author(s) Ortega, J. (Laboratorio de Termodinamica y Fisicoquímica, 35071 - University of Las Palmas de G. C., of table 3k; Canary Islands, Spain)
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Susial, P.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquímica, 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

		P/kPa=101.32		P/kPa=114.66		P/kPa=127.99	
x ₁	T/K	y ₁	T/K	y ₁	T/K	y ₁	
0.00	370.35	0	373.57	0	376.56	0	
0.05	364.17	0.2459	367.69	0.2333	370.91	0.2232	
0.10	359.12	0.4120	362.82	0.3949	366.18	0.3812	
0.15	354.98	0.5276	358.79	0.5098	362.21	0.4954	
0.20	351.56	0.6108	355.42	0.5938	358.88	0.5802	
0.25	348.71	0.6727	352.59	0.6571	356.05	0.6447	
0.30	346.31	0.7202	350.18	0.7062	353.63	0.6952	
0.40	342.48	0.7883	346.33	0.7774	349.74	0.7688	
0.50	339.56	0.8357	343.35	0.8273	346.73	0.8206	
0.60	337.20	0.8722	340.94	0.8660	344.29	0.8607	
0.70	335.18	0.9034	338.87	0.8991	342.21	0.8949	
0.75	334.25	0.9182	337.91	0.9147	341.25	0.9110	
0.80	333.35	0.9329	336.99	0.9302	340.34	0.9271	
0.85	332.46	0.9480	336.09	0.9461	339.44	0.9435	
0.90	331.59	0.9639	335.20	0.9626	338.56	0.9607	
0.95	330.71	0.9810	334.31	0.9804	337.68	0.9793	
1.00	329.82	1	333.41	1	336.79	1	



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_2^2}{T} \right) \right] \quad c_2 = \exp \left[-\left(a_2 + \frac{a_1^2}{T} \right) \right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 x_i P_i^s \exp \left[\frac{\mu_i^E - (B_{ii} - V_i^s)(P - P_i^s) - 2PB_{12}^E(1 - y_2)^2}{RT} \right]$$

$$\mu_1^E = G^E - x_2^2 (\partial G^E / \partial x_2)_{T,P} \quad \mu_2^E = G^E - x_1 (\partial G^E / \partial x_1)_{T,P}$$

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₁ /K	a ₂ /K ²
101.32	211.63 (5.8)	0 (0)	76.75 (4.5)	0 (0)
114.66	208.55 (5.9)	0 (0)	71.83 (4.7)	0 (0)
127.99	223.95 (3.5)	0 (0)	58.57 (2.7)	0 (0)

The std. deviations (σ_a) of the coeffs. a_i are given in parentheses.

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.25347	-2662.78	-53.46	16.11528	-3483.67	-67.34
114.66	14.2531	-2662.78	-53.46	16.11789	-3483.67	-67.34
127.99	14.25011	-2662.78	-53.46	16.11789	-3483.67	-67.34

Std. dev. σ(T)/K, rel. std. dev. 100σ(dP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.091, 0.362, 0.201.
at P/kPa = 114.66 are resp.: 0.088, 0.33, 0.34.
at P/kPa = 127.99 are resp.: 0.05, 0.187, 0.2.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32, 114.66 and 127.99 kPa are reported in ref. 2.
Computations: The 34 T_{exp} data at 101.32 kPa, 35 T_{exp} data at 114.66 kPa and 33 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_i^s (ref. 6).
Errors: Std. dev. σ(T) = [Σ(T - T_{exp})²/(N-n-m)]^{1/2},
Rel. std. dev. 100σ(dP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N-n-m)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. of coefficients in the smoothing equation,
m, no. of exp. points of pure compounds.

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- Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Components: 1. 1-Propanol, C₃H₈O [71-23-8]
 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
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 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

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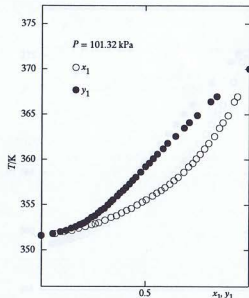
Edited by: Maczyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

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

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32					
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0.0000	351.65	0.0000	0.5762	356.65	0.3945
0.0659	351.85	0.0556	0.5956	356.95	0.4081
0.1094	352.05	0.0916	0.6180	357.35	0.4251
0.1478	352.20	0.1202	0.6384	357.75	0.4404
0.1807	352.45	0.1443	0.6587	358.10	0.4558
0.2120	352.65	0.1657	0.6854	358.65	0.4784
0.2429	352.85	0.1849	0.7091	359.25	0.5017
0.2595	352.95	0.1962	0.7287	359.65	0.5194
0.2774	353.05	0.2073	0.7468	360.15	0.5388
0.3059	353.35	0.2241	0.7650	360.65	0.5592
0.3353	353.65	0.2431	0.7862	361.25	0.5863
0.3609	353.85	0.2580	0.8067	361.85	0.6079
0.3866	354.15	0.2733	0.8343	362.65	0.6456
0.4108	354.45	0.2877	0.8575	363.55	0.6875
0.4341	354.65	0.3025	0.8742	364.15	0.7125
0.4619	355.05	0.3193	0.8990	364.95	0.7503
0.4858	355.35	0.3334	0.9284	366.45	0.8159
0.5052	355.60	0.3450	0.9428	367.05	0.8444
0.5349	356.05	0.3669	1.0000	370.10	1.0000
0.5547	356.35	0.3790			



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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 Gerateman Wertheim) and measured with a mercury manometer.

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 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); $\rho(D, 298.15\text{ K}) = 1.3740$, $\rho(298.15\text{ K})/\text{kg m}^{-3} = 908.53$.

Errors: | $\delta T(\text{estd.})|/\text{K} = 0.01$; | $\delta P(\text{estd.})|/\text{kPa} = 20$; | $\delta x_1| = 0.002$; | $\delta y_1| = 0.01$.

REFERENCES

1. *Int. DATA Ser., Ser. A. Guideline 3k, 1994, 22(4)*.
2. Susial, P.; Ortega, J.; de Alfonso, C.; Alonso, C. *J. Chem. Eng. Data* **1989**, *34*, 247.
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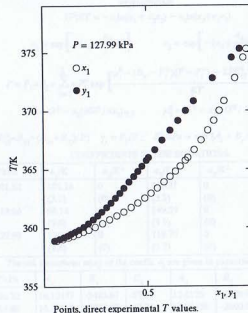
Edited by: Maczynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

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DIRECT EXPERIMENTAL VALUES

P/kPa = 114.66						P/kPa = 127.99					
x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.9790	372.04	0.9380	0.5137	359.75	0.3669	0.9818	375.32	0.9489	0.5197	362.99	0.3685
0.9461	370.53	0.8609	0.4900	359.38	0.3486	0.9666	374.58	0.9110	0.4893	362.57	0.3484
0.9283	369.83	0.8236	0.4604	359.00	0.3291	0.9255	372.81	0.8205	0.4555	362.17	0.3262
0.9093	369.04	0.7907	0.4319	358.62	0.3117	0.8746	370.87	0.7283	0.4229	361.79	0.3050
0.8914	368.34	0.7534	0.3854	358.17	0.2842	0.8506	370.04	0.6894	0.3876	361.40	0.2819
0.8369	366.43	0.6601	0.3498	357.83	0.2625	0.8249	369.19	0.6516	0.3543	361.08	0.2613
0.8214	365.88	0.6410	0.3256	357.54	0.2449	0.7949	368.36	0.6136	0.3187	360.74	0.2396
0.7954	365.13	0.6069	0.2992	357.25	0.2256	0.7635	367.51	0.5755	0.2848	360.41	0.2163
0.7665	364.29	0.5719	0.2636	356.95	0.2060	0.7292	366.71	0.5399	0.2490	360.12	0.1935
0.7326	363.49	0.5365	0.2292	356.62	0.1802	0.6988	366.04	0.5088	0.2185	359.87	0.1712
0.6617	361.98	0.4706	0.2042	356.48	0.1631	0.6869	365.79	0.4984	0.1923	359.69	0.1528
0.6404	361.55	0.4512	0.1702	356.27	0.1398	0.6619	365.30	0.4766	0.1671	359.53	0.1316
0.6185	361.19	0.4350	0.1110	355.95	0.0935	0.6388	364.87	0.4564	0.1434	359.37	0.1159
0.5857	360.59	0.4092	0.0923	355.85	0.0782	0.6122	364.43	0.4364	0.1197	359.24	0.0974
0.5802	360.54	0.4054	0.0797	355.79	0.0665	0.5835	363.94	0.4133	0.0946	359.09	0.0769
0.5612	360.26	0.3941	0.0638	355.75	0.0548	0.5510	363.43	0.3899	0.0635	358.95	0.0524
0.5497	360.04	0.3841									



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 (Normschiff Geratebau 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) = 1.3835, ρ(298.15 K)/kg m⁻³ = 799.65.
 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| = 0.002 and 0.001 at 115 and 128 kPa; |δy₁| = 0.01 and 0.005 at 115 and 128 kPa.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P. *J. Chem. Eng. Jpn.* 1990, 23, 349.
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. 1-Propanol, C₃H₈O [71-23-8]
 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 Termodinámica y Fisicoquímica, 35071 - University of Las Palmas de G. C., of table 3k: Canary Islands, Spain)

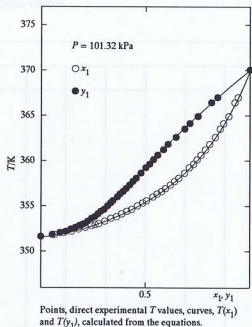
Compiled by: Orac, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Susial, P.; Ortega, J.; de Alfonso, C.; Alonso, C. (Laboratorio de Termodinámica y Fisicoquímica, 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=101.32		P/kPa=114.66		P/kPa=127.99	
	T/K	y ₁	T/K	y ₁	T/K	y ₁
0.00	351.65	0	355.60	0	358.75	0
0.05	351.75	0.0451	355.71	0.0452	358.90	0.0443
0.10	351.95	0.0847	355.90	0.0855	359.12	0.0846
0.15	352.21	0.1203	356.16	0.1222	359.41	0.1218
0.20	352.53	0.1531	356.48	0.1563	359.74	0.1566
0.25	352.90	0.1838	356.84	0.1885	360.12	0.1898
0.30	353.32	0.2133	357.26	0.2195	360.54	0.2219
0.40	354.31	0.2710	358.23	0.2805	361.53	0.2850
0.50	355.53	0.3311	359.43	0.3438	362.73	0.3501
0.60	357.05	0.3990	360.92	0.4148	364.21	0.4222
0.70	359.01	0.4822	362.81	0.5004	366.07	0.5080
0.75	360.21	0.5330	363.96	0.5519	367.20	0.5591
0.80	361.60	0.5927	365.28	0.6115	368.50	0.6181
0.85	363.23	0.6643	366.81	0.6820	370.00	0.6875
0.90	365.14	0.7517	368.58	0.7668	371.75	0.7708
0.95	367.41	0.8609	370.66	0.8706	373.80	0.8728
1.00	370.10	1	373.11	1	376.24	1



EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	101.28 (3.2)	0 (0)	165.31 (3.5)	0 (0)
114.66	98.14 (5.6)	0 (0)	149.59 (5.9)	0 (0)
127.99	120.75 (1.8)	0 (0)	118.75 (1.7)	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
101.32	16.12477	-3483.67	-67.34	13.8173	-2600.93	-68.91
114.66	16.13519	-3483.67	-67.34	13.81424	-2600.93	-68.91
127.99	16.12972	-3483.67	-67.34	13.82563	-2600.93	-68.91

Std. dev. σ(T)/K, rel. std. dev. 100σ(ΔP/P), and abs. max. dev. Δ_m(T)/K at P/kPa = 101.32 are resp.: 0.041, 0.153, 0.14.
 at P/kPa = 114.66 are resp.: 0.06, 0.217, 0.121.
 at P/kPa = 127.99 are resp.: 0.017, 0.062, 0.04.

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32, 114.66 and 127.99 kPa are reported in ref. 2.
Computations: The 39 T_{exp} data at 101.32 kPa, 33 T_{exp} data at 114.66 kPa and 32 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 - m)]^{1/2},
 Rel. std. dev. 100σ(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N - n - m)]^{1/2},
 N, no. of exp. points, ref. 2,
 n, no. of coefficients in the smoothing equation,
 m, no. of exp. points of pure compounds.

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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. 1-Propanol, C₃H₈O [71-23-8]
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: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

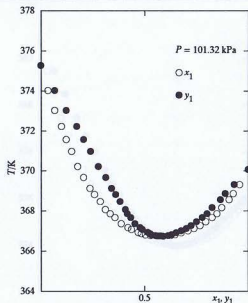
SOURCE OF DATA

Ortega, J.; Susial, P.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., 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	375.30	0.0000	0.5051	366.83	0.5338
0.0335	374.05	0.0661	0.5286	366.80	0.5519
0.0664	373.05	0.1213	0.5599	366.79	0.5695
0.0981	372.25	0.1716	0.5756	366.78	0.5793
0.1221	371.60	0.2057	0.5913	366.77	0.5910
0.1473	371.00	0.2395	0.6255	366.80	0.6145
0.1771	370.25	0.2776	0.6484	366.85	0.6311
0.2066	369.70	0.3122	0.6766	366.95	0.6525
0.2362	369.15	0.3400	0.7087	367.05	0.6773
0.2590	368.85	0.3594	0.7385	367.15	0.7008
0.2856	368.50	0.3815	0.7673	367.30	0.7243
0.3102	368.10	0.4080	0.7957	367.50	0.7500
0.3344	367.90	0.4174	0.8258	367.70	0.7786
0.3572	367.70	0.4335	0.8486	367.90	0.8008
0.3872	367.40	0.4540	0.8722	368.20	0.8257
0.4200	367.20	0.4792	0.9082	368.60	0.8661
0.4362	367.10	0.4892	0.9270	368.90	0.8895
0.4690	366.97	0.5155	0.9581	369.35	0.9327
0.4840	366.90	0.5263	1.0000	370.10	1.0000



Points, direct experimental T values.

AUXILIARY INFORMATION

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

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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) = 1.3835, ρ(298.15 K)/kg·m⁻³ = 799.65.
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(Std.)|/K = 0.01; |δP(Std.)|/Pa = 20; |δx₁| = 0.001; |δy₁| = 0.005.

REFERENCES

1. Int. DATA Ser., Ser. A, *Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P.; de Alfonso, C. *J. Chem. Eng. Data* 1990, 35, 216.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

Received: February 28, 1995

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

Published: April 30, 1995

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

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2. Methyl butanoate, $C_5H_{10}O_2$ [623-42-7]
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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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)

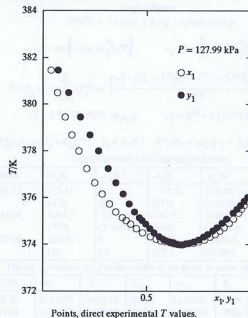
Edited by: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

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

$P/kPa = 114.66$						$P/kPa = 127.99$											
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1						
0.9583	372.44	0.9334	0.5060	371.07	0.5526	0.9928	376.04	0.9854	0.6156	374.10	0.6292						
0.9360	372.17	0.9041	0.4785	371.20	0.5321	0.9816	375.87	0.9689	0.5924	374.13	0.6128						
0.9282	372.11	0.8950	0.4461	371.33	0.5114	0.9696	375.70	0.9516	0.5697	374.17	0.5976						
0.9112	371.93	0.8745	0.4215	371.50	0.4910	0.9568	375.53	0.9351	0.5473	374.24	0.5821						
0.8837	371.68	0.8443	0.3934	371.70	0.4692	0.9425	375.36	0.9162	0.5178	374.35	0.5615						
0.8701	371.58	0.8298	0.3595	371.93	0.4457	0.9187	375.10	0.8866	0.4809	374.51	0.5364						
0.8497	371.40	0.8083	0.3316	372.19	0.4228	0.8981	374.92	0.8642	0.4520	374.69	0.5166						
0.8273	371.28	0.7873	0.3013	372.51	0.3965	0.8736	374.73	0.8393	0.4240	374.88	0.4967						
0.8099	371.20	0.7716	0.2456	373.24	0.3422	0.8545	374.60	0.8196	0.4026	375.04	0.4806						
0.7845	371.09	0.7499	0.2157	373.71	0.3113	0.8311	374.44	0.7960	0.3844	375.16	0.4668						
0.7564	370.99	0.7268	0.1898	374.11	0.2825	0.8058	374.33	0.7750	0.3528	375.41	0.4429						
0.7282	370.90	0.7057	0.1670	374.53	0.2552	0.7794	374.21	0.7517	0.3216	375.75	0.4170						
0.7146	370.88	0.6964	0.1460	374.96	0.2293	0.7530	374.13	0.7298	0.2857	376.17	0.3870						
0.6874	370.87	0.6772	0.1229	375.49	0.1981	0.7279	374.08	0.7097	0.2501	376.66	0.3523						
0.6631	370.85	0.6617	0.0992	376.04	0.1656	0.7018	374.04	0.6902	0.2127	377.26	0.3148						
0.6454	370.84	0.6478	0.0757	376.72	0.1280	0.6778	374.01	0.6725	0.1738	378.02	0.2698						
0.6201	370.86	0.6309	0.0563	377.35	0.0919	0.6631	374.00	0.6620	0.1405	378.70	0.2275						
0.5909	370.87	0.6135	0.0306	378.09	0.0525	0.6491	374.02	0.6518	0.1084	379.47	0.1819						
0.5630	370.91	0.5944	0.0115	378.71	0.0173	0.6344	374.04	0.6418	0.0712	380.51	0.1245						
0.5336	370.99	0.5727				0.6173	374.09	0.6298	0.0402	381.48	0.0738						



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. High purity nitrogen was used for the backing pressure.
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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); $n(D, 298.15\text{ K}) = 1.3851$, $\rho(298.15\text{ K}) = 892.37$.
Errors: $|\delta T(\text{estd.})|/K = 0.01$; $|\delta P(\text{estd.})|/kPa = 20$; $|\delta x_i| = 0.001$; $|\delta y_i| = 0.005$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Susial, P. *Can. J. Chem. Eng.* 1991, 69, 394.
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 2. Methyl butanone, 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
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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)

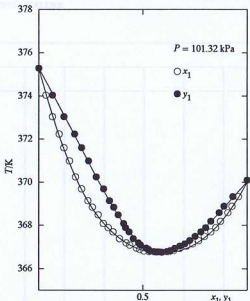
SOURCE OF DATA

Ortega, J.; Susial, P.; de Alfonso, C. (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

P/kPa=101.32		P/kPa=114.66		P/kPa=127.99	
x ₁	T/K	y ₁	T/K	y ₁	T/K
0.00	375.30	0	379.14	0	382.84
0.05	373.64	0.0939	377.44	0.0941	381.07
0.10	372.15	0.1753	376.04	0.1730	379.64
0.15	370.87	0.2445	374.89	0.2401	378.46
0.20	369.80	0.3031	373.95	0.2981	377.49
0.25	368.95	0.3529	373.18	0.3491	376.69
0.30	368.27	0.3961	372.56	0.3946	376.04
0.40	367.36	0.4692	371.65	0.4746	375.06
0.50	366.89	0.5333	371.10	0.5458	374.43
0.60	366.76	0.5964	370.84	0.6144	374.10
0.70	366.95	0.6656	370.84	0.6860	374.03
0.75	367.19	0.7048	370.95	0.7249	374.11
0.80	367.52	0.7486	371.15	0.7671	374.27
0.85	367.96	0.7984	371.43	0.8139	374.52
0.90	368.53	0.8556	371.83	0.8669	374.91
0.95	369.24	0.9221	372.37	0.9280	375.46
1.00	370.10	1.0000	373.07	1.0000	376.23

Sid. dev. σ(T)/K, rel. sid. dev. 100σ(ΔP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.027, 0.089, 0.097.
 at P/kPa = 114.66 are resp.: 0.022, 0.076, 0.058.
 at P/kPa = 127.99 are resp.: 0.038, 0.128, 0.11.



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_1^2}{T} \right) / T \right] \quad c_2 = \exp \left[-\left(a_2 + \frac{a_2^2}{T} \right) / T \right]$$

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	175.15 (4.3)	0 (0)	-778.75 (115)	318690 (44100)
114.66	4293.7 (733)	-1522600 (274000)	-2817.1 (418)	1068600 (157000)
127.99	153.33 (2)	0 (0)	-3673 (121)	1405700 (45200)

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
101.32	16.12477	-3483.67	-67.34	14.07885	-2926.72	-65.94
114.66	16.13668	-3483.67	-67.34	14.08654	-2926.72	-65.94
127.99	16.13009	-3483.67	-67.34	14.08742	-2926.72	-65.94

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32, 114.66 and 127.99 kPa are reported in ref. 2.
Computations: The 38 T_{exp} data at 101.32 kPa, 39 T_{exp} data at 114.66 kPa and 40 T_{exp} data at 127.99 kPa were reduced using the modified Wilson eq., ref. 3, for the partial molar excess for the partial molar excess Gibbs energy 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-m)]^{1/2},
 Rel. sid. dev. 100σ(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N-n-m)]^{1/2},
 N, no. of exp. points, ref. 2,
 n, no. of coefficients in the smoothing equation,
 m, no. of exp. points of pure compounds.

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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. 1-Propanol, C_3H_8O [71-23-8]
 2. Ethyl ethanoate, $C_4H_8O_2$ [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) Ortega, J. (Laboratorio de Termodinámica y Físicoquímica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)

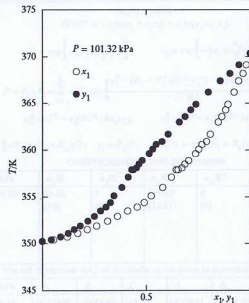
Edited by: Maczyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (Laboratorio de Termodinámica y Físicoquímica, 35071 - University of Las Palmas de G. C., 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	350.30	0.0000	0.6856	358.55	0.4660
0.0539	350.45	0.0438	0.7040	358.95	0.4820
0.1194	350.75	0.0879	0.7386	359.65	0.5156
0.1705	351.15	0.1243	0.7540	360.15	0.5320
0.2174	351.55	0.1546	0.7691	360.65	0.5495
0.2611	351.95	0.1838	0.7902	360.95	0.5771
0.3140	352.45	0.2198	0.8099	361.75	0.6066
0.3621	352.95	0.2511	0.8482	363.05	0.6596
0.4114	353.55	0.2794	0.8643	363.65	0.6884
0.4565	353.95	0.3065	0.8835	364.35	0.7161
0.4914	354.45	0.3274	0.8938	364.95	0.7401
0.5245	355.15	0.3445	0.9227	366.25	0.7994
0.5798	356.05	0.3835	0.9453	367.45	0.8568
0.6219	357.15	0.4138	0.9661	368.25	0.9034
0.6442	357.95	0.4309	0.9816	369.15	0.9465
0.6531	357.95	0.4381	1.0000	370.40	1.0000
0.6722	358.15	0.4536			



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 ± 0.1 K with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa.

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); $n(D, 298.15 \text{ K}) = 1.3833$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 799.54$.
 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); $n(D, 298.15 \text{ K}) = 1.3699$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 894.34$.

Errors: $|\delta T(\text{estd.})|/K = 0.1$; $|\delta P(\text{estd.})|/Pa = 70$; $|\delta x_1| = 0.005$; $|\delta y_1| = 0.01$.

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Int. DATA Ser., Ser. A 1995, 23(2), 102-122

Received: February 28, 1995

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

Published: April 30, 1995

0147-1503/95/0902-111\$2.20

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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. 1-Propanol, C_3H_8O [71-23-8]
2. Ethyl ethanoate, $C_4H_8O_2$ [141-78-6]

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)

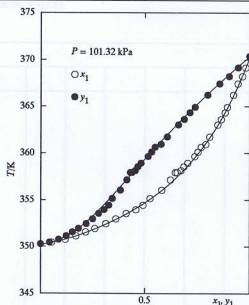
SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (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 y_1

x_1	$P/kPa = 101.32$		y_1				
	T/K	y_1					
0.00	350.30	0.					
0.05	350.47	0.0429					
0.10	350.72	0.0802					
0.15	351.05	0.1135					
0.20	351.43	0.1441					
0.25	351.85	0.1729					
0.30	352.33	0.2006					
0.40	353.43	0.2558					
0.50	354.79	0.3145					
0.60	356.47	0.3824					
0.70	358.63	0.4672					
0.75	359.95	0.5195					
0.80	361.46	0.5812					
0.85	363.21	0.6552					
0.90	365.25	0.7456					
0.95	367.62	0.8580					
1.00	370.40	1					

Sid. dev. $\sigma(T)/K$, rel. std. dev. $100\sigma(\delta P/P)$, and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.33$ are resp.: 0.171, 0.644, 0.532.



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

EQUATIONS

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

$$c_1 = \exp\left[-\left(a_1 + \frac{a_1^2}{T}\right)/T\right] \quad c_2 = \exp\left[-\left(a_2 + \frac{a_2^2}{T}\right)/T\right]$$

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
101.33	68.06 (10)	0 (0)	199.42 (12.6)	0 (0)

The std. deviations $\sigma(a_i)$ of the coeffs. a_i are given in parantheses.

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.33	16.11348	-3483.67	-67.34	14.12011	-2751.89	-60.68

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 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_i^0 (ref. 6).

Errors: Sid. dev. $\sigma(T) = [\Sigma(T - T_{exp})^2/(N-n-2)]^{1/2}$,
Rel. std. dev. $100\sigma(\delta P/P) = 100[\Sigma((P - P_{exp})/P_{exp})^2/(N-n-2)]^{1/2}$,
 N , no. of exp. points, ref. 2,
 n , no. of coefficients in the smoothing equation.

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5. Tsouopoulos, C. *AIChE J.* 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. *AIChE J.* 1966, 12, 95.

Components: 1. 1-Propanol, C₃H₈O [71-23-8]
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: 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)

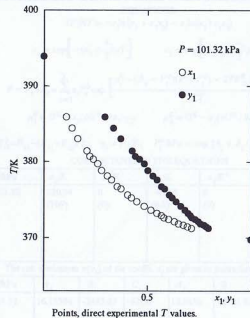
Edited by: Maczyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., 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	394.00	0.0000	0.4238	375.30	0.6195														
0.1077	386.00	0.2941	0.4494	374.80	0.6380														
0.1360	384.50	0.3349	0.4849	374.20	0.6614														
0.1638	383.10	0.3714	0.5169	373.70	0.6817														
0.2070	381.50	0.4261	0.5454	373.30	0.6964														
0.2212	380.80	0.4420	0.5678	373.00	0.7078														
0.2390	380.40	0.4615	0.5798	372.70	0.7160														
0.2597	379.80	0.4840	0.6034	372.50	0.7304														
0.2782	378.90	0.5018	0.6314	372.20	0.7466														
0.3058	378.20	0.5267	0.6507	371.90	0.7569														
0.3267	377.70	0.5454	0.6742	371.70	0.7744														
0.3545	376.80	0.5681	0.6946	371.50	0.7844														
0.3725	376.50	0.5826	0.7136	371.30	0.7958														
0.4050	375.70	0.6059	1.0000	370.40	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 (Normschiff Geratebau Wertheim) and measured with a mercury manometer.

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.1 K with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); ρ(298.15 K)/kg·m⁻³ = 799.54.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mole %, treated with calcium chloride, dried with potassium carbonate, and fractionally dist. through a 120-plate lab. column; degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); ρ(298.15 K)/kg·m⁻³ = 873.75.

Errors: |δT(estd.)|/K = 0.1; |δP(estd.)|/Pa = 70; |δx₁| = 0.002; |δy₁| = 0.01.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
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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. 1-Propanol, C₃H₈O [71-23-8]
2. Ethyl butanoate, C₈H₁₆O₂ [105-54-4]
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 3c Canary Islands, Spain)

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

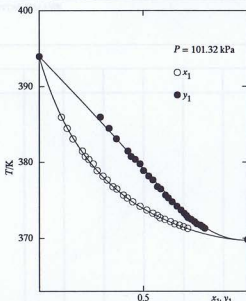
SOURCE OF DATA

Ortega, J.; Pena, J. A.; de Alfonso, C. (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

P/kPa=101.32						
x ₁	T/K	y ₁				
0.00	394.00	0				
0.05	389.82	0.1467				
0.10	386.55	0.2579				
0.15	383.90	0.3459				
0.20	381.71	0.4178				
0.25	379.88	0.4781				
0.30	378.32	0.5297				
0.40	375.83	0.6147				
0.50	373.96	0.6835				
0.60	372.53	0.7429				
0.70	371.44	0.7979				
0.75	371.00	0.8253				
0.80	370.62	0.8535				
0.85	370.30	0.8835				
0.90	370.05	0.9166				
0.95	369.88	0.9545				
1.00	369.83	1				

Std. dev. α(T)/K, rel. std. dev. 100α(ΔP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.087, 0.273, 0.24.



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_2^2}{T} \right) / T \right] \quad c_2 = \exp \left[-\left(a_3 + \frac{a_4}{T} \right) / T \right]$$

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

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

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad y_1 = P_1/P; \quad P_i^0/kPa = \exp [A_i + B_i / (C_i + T/K)]$$

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	310.94 (109)	0 (0)	-43.18 (6.5)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	16.13504	-3483.67	-67.34	12.1636	-2121.97	-112.77

AUXILIARY INFORMATION

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

Computations: The 28 T_{exp} data at 101.32 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 imperfections 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. α(T) = [Σ(T - T_{exp})² / (N - n)]^{1/2},
Rel. std. dev. 100α(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})² / (N - n)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. of coefficients in the smoothing equation.

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2. Ortega, J. *Int. DATA Ser. Ser. A. Data Mixtures*, Ser. A 1995, 23, 113.
3. Wilson, G. M. *J. Am. Chem. Soc.* 1964, 86, 127.
4. *TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons*, 1976, k-5000, 1978, k-5620, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsouopoulos, 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. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl methanoate, C₄H₈O₂ [110-74-7]
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

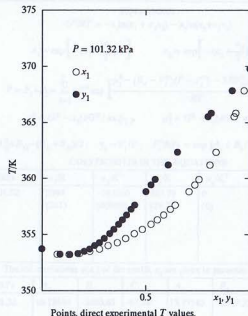
Author(s) of table: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)
Edited by: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Galvan, S.; Ortega, J.; Susial, P.; Pena, J. A. (Laboratorio de Termodinamica y Fisicoquimica, 35071 - University of Las Palmas de G. C., 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	353.79	0.0000	0.5879	356.78	0.4098
0.0735	353.30	0.0874	0.6206	357.28	0.4313
0.1302	353.27	0.1347	0.6425	357.67	0.4483
0.1819	353.36	0.1731	0.7096	358.88	0.5013
0.2322	353.55	0.2050	0.7365	359.48	0.5257
0.2781	353.76	0.2300	0.7573	359.95	0.5457
0.3196	354.05	0.2557	0.8088	361.25	0.6098
0.3646	354.33	0.2779	0.8381	362.38	0.6546
0.4053	354.68	0.3019	0.9252	365.55	0.8002
0.4464	355.11	0.3270	0.9329	365.88	0.8148
0.4844	355.48	0.3474	0.9724	367.88	0.9160
0.5260	355.96	0.3711	1.0000	369.83	1.0000
0.5563	356.35	0.3900			



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 (Normschiff 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 > 99.8 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); n(D, 298.15 K) = 1.3833, ρ(298.15 K)/kg·m⁻³ = 799.54.
2. Aldrich Chemicals Co., Inc. (Milwaukee, WI, USA), highest commercial purity grade material, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); n(D, 298.15 K) = 1.3747, ρ(298.15 K)/kg·m⁻³ = 899.22.
Errors: |δT(estd.)|/K = 0.02; |δP(estd.)|/kPa = 20; |δx₁| = 0.001; |δy₁| = 0.015.

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2. Galvan, S.; Ortega, J.; Susial, P.; Pena, J. A. *J. Chem. Eng. Jpn.* 1994, 27, 529.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

0147-1303/95/0502-11\$5.20

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Int. DATA Ser., Ser. A 1995, 23(5), 102-122

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Received: February 28, 1995

Published: April 30, 1995

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. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl methanoate, C₄H₈O₂ [110-74-7]

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 x₂ and constant P; ref. 1

Author(s) of table 3k: Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., Canary Islands, Spain)

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

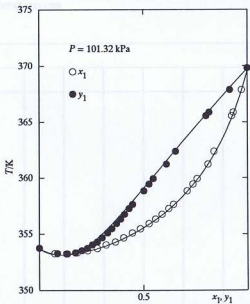
SOURCE OF DATA

Galvan, S.; Ortega, J.; Susial, P.; Pena, J. A. (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

P/kPa = 101.32					
x ₁	T/K	y ₁			
0.00	353.79	0			
0.05	353.37	0.0587			
0.10	353.24	0.1025			
0.15	353.28	0.1381			
0.20	353.42	0.1689			
0.25	353.64	0.1971			
0.30	353.92	0.2238			
0.40	354.66	0.2766			
0.50	355.65	0.3332			
0.60	356.96	0.3985			
0.70	358.70	0.4789			
0.75	359.79	0.5279			
0.80	361.07	0.5852			
0.85	362.59	0.6540			
0.90	364.45	0.7391			
0.95	366.77	0.8491			
1.00	369.83	1			

Std. dev. σ(T)/K, rel. std. dev. 100σ(ΔP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.057, 0.218, 0.18.



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

EQUATIONS

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

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

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	2094 (241)	-743800 (40900)	359.79 (24.2)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	1613504	-3483.67	-67.34	13.77542	-2607.22	-69.07

AUXILIARY INFORMATION

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

Computations: The 25 T_{exp} data at 101.32 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.

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2. Ortega, J. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23, 115.
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01471-1503/95/095020-11\$02.20

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Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2), 102-122

Received: February 28, 1995

Published: April 30, 1995

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. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl ethanoate, C₆H₁₄O₂ [109-60-4]
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: Direct measurement of T, x_i, and y_i at constant P; ref. 1

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

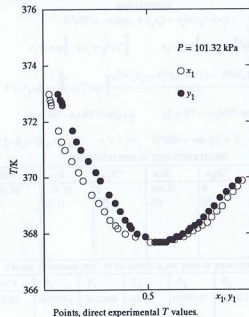
Edited by: Mączyski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. (Laboratorio de Termodinámica y Fisicoquímica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32					
x ₁	T/K	y ₁	x ₁	T/K	y ₁
0.0290	373.0	0.0722	0.5338	367.7	0.5530
0.0343	372.8	0.0830	0.5645	367.7	0.5744
0.0383	372.7	0.0906	0.5876	367.7	0.5915
0.0403	372.6	0.0946	0.6112	367.8	0.6074
0.0732	371.7	0.1413	0.6302	367.8	0.6220
0.0882	371.3	0.1606	0.6541	367.9	0.6394
0.1050	371.0	0.1809	0.6757	367.9	0.6559
0.1364	370.6	0.2170	0.6951	368.0	0.6709
0.1688	370.2	0.2520	0.7194	368.1	0.6991
0.1911	369.9	0.2744	0.7430	368.2	0.7083
0.2326	369.4	0.3147	0.7646	368.3	0.7291
0.2642	369.1	0.3439	0.7886	368.4	0.7508
0.2921	368.8	0.3686	0.8110	368.6	0.7724
0.3187	368.5	0.3918	0.8360	368.8	0.7973
0.3455	368.3	0.4135	0.8608	369.0	0.8227
0.3563	368.2	0.4215	0.8872	369.3	0.8503
0.3923	368.0	0.4497	0.9139	369.5	0.8808
0.4412	367.9	0.4895	0.9357	369.7	0.9103
0.5116	367.7	0.5385	0.9591	369.9	0.9405



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 Geratbau Wertheim) and measured with a mercury manometer.
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.1 K with a digital thermometer, Bailey Instruments, calibrated against IPTS-68. Compositions were determined by densimetric analysis, using a Anton Paar, Model DMA-55 vibrating-tube digital densimeter. Pressure was maintained constant to within 0.07 kPa.
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); ρ(298.15 K)/kg m⁻³ = 799.54.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 95 mole %, washed with sodium carbonate, treated with calcium chloride, dried with potassium carbonate, and fractionally, distd. through a 120-plate lab. column; degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 4A (Fluka AG); ρ(298.15 K)/kg m⁻³ = 880.97.
Errors: |δT(estd.)|/K = 0.1; |δP(estd.)|/Pa = 70; |δx₁| = 0.005; |δy₁| = 0.008.

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2. Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. *Can. J. Chem. Eng.* 1987, 65, 982.
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. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl ethanoate, C₅H₁₀O₂ [109-64-4]
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 Fisicoquímica, 35071-University of Las Palmas de G. C., Orta de las Palmas, Canary Islands, Spain)
Of table 3c

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

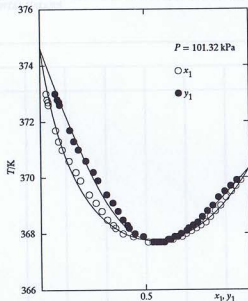
SOURCE OF DATA

Ortega, J.; Ocon, J.; Pena, J. A.; de Alfonso, C.; Paz-Andrade, M. I.; Fernandez, J. (Laboratorio de Termodinamica y Fisicoquímica, 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

P/kPa=101.32				
x ₁	T/K	y ₁		
0.00	374.64	0		
0.05	372.59	0.1031		
0.10	371.20	0.1786		
0.15	370.21	0.2381		
0.20	369.49	0.2875		
0.25	368.95	0.3307		
0.30	368.54	0.3699		
0.40	368.03	0.4421		
0.50	367.80	0.5122		
0.60	367.82	0.5855		
0.70	368.06	0.6664		
0.75	368.28	0.7109		
0.80	368.56	0.7590		
0.85	368.90	0.8111		
0.90	369.32	0.8682		
0.95	369.82	0.9308		
1.00	370.40	1		

Std. dev. α(T)/K, rel. std. dev. 100α(ΔP/P), and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.159, 0.516, 0.33.



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_2^2}{T} \right) / T \right] \quad c_2 = \exp \left[-\left(a_2 + \frac{a_1^2}{T} \right) / T \right]$$

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₁ /K	a ₂ /K ²
101.32	-10.71 (4.2)	0 (0)	300.33 (5)	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
101.32	16.05311	-3452.06	-68.51	13.94327	-2840.15	-70.07

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.
Computations: The 38 T_{exp} data at 101.32 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_i^s (ref. 6).
Errors: Std. dev. α(T) = [Σ(T - T_{exp})²/(N-n)]^{1/2}.
Rel. std. dev. 100α(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})²/(N-n)]^{1/2}.
N, no. of exp. points, ref. 2.
n, no. of coefficients in the smoothing equation.

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1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Ser. Data Mixtures, Ser. A 1995, 23, 117.
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5. Tsoumpoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.
6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.

Published by Thermodynamics Research Center

Components: 1. 1-Propanol, C_3H_8O [71-23-8]
2. Propyl propanoate, $C_6H_{12}O_2$ [106-36-5]

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_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)

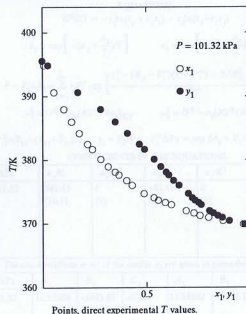
Edited by: Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., 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	395.65	0.0000	0.4319	376.13	0.6579												
0.0080	394.95	0.0275	0.4885	374.78	0.7035												
0.0570	390.69	0.1716	0.5363	374.16	0.7219												
0.1043	388.05	0.2810	0.5591	373.76	0.7349												
0.1423	386.06	0.3523	0.5930	373.40	0.7525												
0.1789	384.26	0.4104	0.6217	373.03	0.7647												
0.2190	382.53	0.4672	0.6930	372.06	0.8043												
0.2421	381.75	0.4922	0.7294	371.75	0.8230												
0.2822	380.17	0.5378	0.7589	371.35	0.8448												
0.3512	378.15	0.5972	0.8689	370.53	0.8998												
0.3698	377.73	0.6086	0.9671	369.96	0.9741												
0.4058	376.88	0.6330	1.0000	369.83	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 ensured 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 Gerateman 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 having a precision of ± 0.02 kg·m⁻³. 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 > 99.8 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3833$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 799.54$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss p.a." grade material, purity > 99 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3918$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 875.65$.

Errors: $|\delta T(\text{estd.})|/K = 0.05$; $|\delta P(\text{estd.})|/kPa = 70$; $|\delta x_1| = 0.002$; $|\delta y_1| = 0.008$.

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

Components: 1. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl propanoate, C₆H₁₂O₂ [106-36-5]

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., Canary Islands, Spain)

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

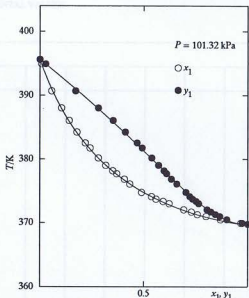
SOURCE OF DATA

Ortega, J.; Galvan, S. (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

P/kPa=101.32		
x ₁	T/K	y ₁
0.00	395.65	0
0.05	391.57	0.1530
0.10	388.28	0.2698
0.15	385.55	0.3621
0.20	383.26	0.4372
0.25	381.31	0.4997
0.30	379.63	0.5528
0.40	376.92	0.6388
0.50	374.84	0.7070
0.60	373.23	0.7644
0.70	371.98	0.8162
0.75	371.45	0.8415
0.80	370.99	0.8673
0.85	370.59	0.8945
0.90	370.25	0.9243
0.95	369.99	0.9586
1.00	369.83	1

Std. dev. σ(T)/K, rel. std. dev. 100σ(ΔP/P)%, and abs. max. dev. δ_m(T)/K at P/kPa = 101.32 are resp.: 0.12, 0.394, 0.36.



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

EQUATIONS

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

$$c_1 = \exp \left[-(a_1 + \frac{a_1^2}{T}) \right] \quad c_2 = \exp \left[-(a_2 + \frac{a_2^2}{T}) \right]$$

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	341.43 (16.1)	0 (0)	-62.66 (9)	0 (0)

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

P/kPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	16.13504	-3483.67	-67.34	14.84882	-3558.18	-47.85

AUXILIARY INFORMATION

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

Computations: The 26 T_{exp} data at 101.32 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 - 2)]^{1/2},
Rel. std. dev. 100σ(ΔP/P) = 100[Σ((P - P_{exp})/P_{exp})² / (N - 2)]^{1/2},
N, no. of exp. points, ref. 2,
n, no. of coefficients in the smoothing equation.

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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. 1-Propanol, C_3H_8O [71-23-8]
2. Propyl butanoate, $C_7H_{14}O_2$ [105-66-8]
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^s , 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)

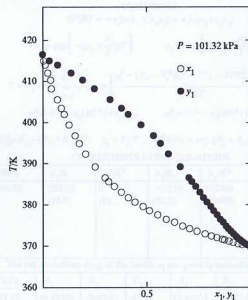
SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinamica y Fisicoquimica, 35071-University of Las Palmas de G. C., 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	416.65	0.0000	0.4452	380.75	0.7912
0.0048	415.05	0.0324	0.4834	379.70	0.8097
0.0119	414.07	0.0720	0.5133	378.70	0.8230
0.0253	412.15	0.1374	0.5534	377.65	0.8404
0.0384	410.45	0.1925	0.5960	376.55	0.8556
0.0420	408.35	0.2486	0.6359	375.85	0.8690
0.0713	405.65	0.3239	0.6741	374.97	0.8824
0.0889	403.55	0.3803	0.7076	374.33	0.8937
0.1038	402.13	0.4123	0.7427	373.73	0.9056
0.1264	399.50	0.4732	0.7809	373.10	0.9179
0.1558	396.85	0.5333	0.8126	372.53	0.9285
0.1754	394.99	0.5675	0.8385	372.15	0.9372
0.2054	392.42	0.6065	0.8645	371.74	0.9463
0.2521	389.31	0.6625	0.8748	371.63	0.9502
0.3004	386.69	0.7044	0.8965	371.29	0.9579
0.3167	385.72	0.7179	0.9163	370.99	0.9659
0.3448	384.55	0.7367	0.9406	370.65	0.9755
0.3790	383.15	0.7576	0.9593	370.40	0.9833
0.4121	381.85	0.7745	1.0000	369.83	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 Vakuumat electronic instrument (Normschiff 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 > 99.8 mole %, degassed ultrasonically before use and stored in the dark for several days over molecular sieves type 3A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3833$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 799.54$.
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 3A (Fluka AG); $n(D, 298.15 \text{ K}) = 1.3976$, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3} = 868.07$.
Errors: $|\delta T(\text{std.})|/K = 0.05$; $|\delta P(\text{std.})|/Pa = 70$; $|\delta x_i| = 0.002$; $|\delta y_i| = 0.03$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 3k*, 1994, 22(4).
2. Ortega, J.; Galvan, S. *J. Chem. Eng. Data* in press.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. *J. Chem. Eng. Data* 1986, 31, 339.

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Int. DATA Ser., Ser. A 1995, 23(3), 102-122

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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. 1-Propanol, C₃H₈O [71-23-8]
2. Propyl butanoate, C₇H₁₄O₂ [105-66-8]
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_i, pressure
Method: Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp}, data at variable x_i and constant P; ref. 1

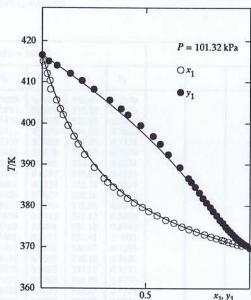
Author(s) Ortega, J. (Laboratorio de Termodinámica y Físicoquímica, 35071 - University of Las Palmas de G. C., Canary Islands, Spain)
Compiled by: Oracz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Galvan, S. (Laboratorio de Termodinámica y Físicoquímica, 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

P/kPa=101.32			
x ₁	T/K	y ₁	
0.00	416.65	0	
0.05	408.63	0.2252	
0.10	402.27	0.3811	
0.15	397.16	0.4926	
0.20	393.00	0.5751	
0.25	389.58	0.6379	
0.30	386.73	0.6871	
0.40	382.31	0.7594	
0.50	379.04	0.8110	
0.60	376.53	0.8515	
0.70	374.50	0.8865	
0.75	373.61	0.9033	
0.80	372.77	0.9201	
0.85	371.99	0.9376	
0.90	371.24	0.9562	
0.95	370.52	0.9767	
1.00	369.83	1	



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

EQUATIONS

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

$$c_1 = \exp \left[-\left(a_1 + \frac{a_2^2}{T} \right) / T \right] \quad c_2 = \exp \left[-\left(a_3 + \frac{a_4}{T} \right) / T \right]$$

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

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

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

COEFFICIENTS IN THE EQUATIONS

P/kPa	a ₁ /K	a ₂ /K ²	a ₃ /K	a ₄ /K ²
101.32	238.32 (15.7)	0 (0)	-952.56 (93.3)	355700 (39900)

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
101.32	16.13504	-3483.67	-67.34	12.44054	-2347.46	-116.55

Std. dev. σ(T)/K, rel. std. dev. 100σ(ΔP/P), and abs. max. dev. δ_{sm}(T)/K at P/kPa = 101.32 are resp.: 0.174, 0.483, 1.307.

AUXILIARY INFORMATION

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

Computations: The 38 T_{exp} data at 101.32 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.

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