

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3k. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

0147-1503/02-81\$4.00

**Components:** 1. Methyl ethanoate,  $C_3H_6O_2$  [79-20-9]  
2. 2-Butanol,  $C_4H_{10}O$  [78-92-2]

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

**Variables:**  $T$ , temperature

$x_i$ , mole fraction of component  $i$  in liquid phase

$y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

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

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

## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

 $P/kPa = 74.66$  $P/kPa = 101.32$ 

$x_1$	$T/K$	$y_1$									
0.0000	364.04	0.0000	0.4300	334.50	0.8257	0.0000	372.36	0.0000	0.6738	337.27	0.8967
0.0144	362.19	0.0787	0.4838	332.80	0.8517	0.0203	369.82	0.0987	0.7601	335.16	0.9257
0.0231	361.16	0.1213	0.5491	331.00	0.8765	0.0260	369.20	0.1220	0.8066	333.89	0.9416
0.0485	358.52	0.2344	0.5899	329.63	0.8934	0.0561	366.39	0.2347	0.8573	332.81	0.9563
0.0789	355.40	0.3464	0.6462	328.37	0.9090	0.1313	360.10	0.4463	0.8988	331.90	0.9695
0.0959	353.80	0.3971	0.7095	326.97	0.9236	0.1564	358.20	0.4980	0.9423	330.92	0.9829
0.1098	352.56	0.4369	0.7692	325.49	0.9407	0.1805	356.58	0.5437	0.9699	330.34	0.9908
0.1255	351.13	0.4778	0.8171	324.23	0.9546	0.2029	355.07	0.5813	1.0000	329.81	1.0000
0.1369	350.12	0.5049	0.8730	323.38	0.9668	0.2444	352.40	0.6405			
0.1532	349.06	0.5341	0.9169	322.53	0.9776	0.2679	351.11	0.6693			
0.1732	347.43	0.5740	0.9526	321.90	0.9867	0.2968	349.48	0.6991			
0.1923	346.10	0.6055	1.0000	321.12	1.0000	0.3205	348.33	0.7210			
0.2145	344.55	0.6397				0.3430	347.28	0.7401			
0.2367	343.30	0.6697				0.3669	346.30	0.7577			
0.2764	341.00	0.7157				0.4023	344.98	0.7817			
0.3144	339.22	0.7500				0.4232	344.35	0.7918			
0.3533	337.34	0.7800				0.4623	342.95	0.8149			
0.3794	336.26	0.7977				0.5129	341.53	0.8375			
0.4047	335.37	0.8118				0.6119	338.52	0.8811			

## AUXILIARY INFORMATION

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

**Procedure:** The procedure was described in ref. 3. The compositions were determined by measuring their densities at  $298.15\text{ K}$  with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of  $\pm 0.02\text{ kg}\cdot\text{m}^{-3}$ . A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition were  $\pm 0.002$  mole fraction for liquid phase and  $\pm 0.004$  mole fraction for vapor phase.

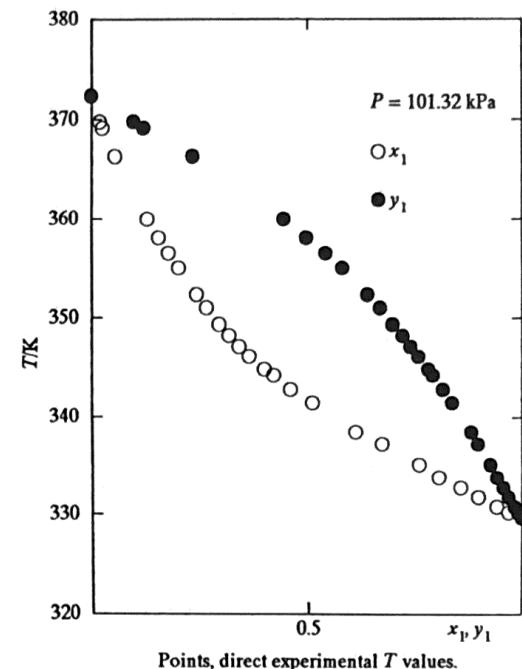
**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $n(D, 298.15\text{ K}) = 1.3590$ ,  $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 927.07$ ; ref. 4.

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $n(D, 298.15\text{ K}) = 1.3949$ ,  $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 802.29$ .

**Errors:**  $|8T|/K = 0.01$ ;  $|8P|/\text{Pa} = 10$ ;  $|8x_1| = 0.003$ ;  $|8y_1| = 0.005$ .

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
2. Ortega, J.; Hernández, P. Fluid Phase Equilib., 1996, 118, 249.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.
4. Ortega, J.; Peña, J. A. J. Chem. Eng. Jpn., 1994, 27, 351.



## SELECTED DATA ON MIXTURES

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## 3k. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

0147-1503/02-8224-00

Components:	1. Methyl ethanoate, $C_3H_6O_2$ [79-20-9] 2. 2-Butanol, $C_4H_{10}O$ [78-92-2]
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	$T$ , temperature $x_i$ , mole fraction of component $i$ in liquid phase $y_i$ , mole fraction of component $i$ in vapor phase
Parameters:	$P$ , pressure
Method:	Direct measurement of $T$ , $x_i$ and $y_i$ at constant $P$ ; ref. 1

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

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

## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

 $P/kPa = 127.99$ 

$x_1$	$T/K$	$y_1$	$x_1$	$T/K$	$y_1$														
0.0000	378.56	0.0000	0.6048	345.90	0.8686														
0.0152	377.19	0.0670	0.6337	344.98	0.8800														
0.0304	375.95	0.1135	0.6640	344.06	0.8910														
0.0461	374.83	0.1615	0.6899	343.57	0.9004														
0.0863	371.83	0.2763	0.7249	342.70	0.9133														
0.1066	370.42	0.3294	0.7597	342.26	0.9238														
0.1300	368.80	0.3831	0.8002	341.29	0.9383														
0.1585	366.87	0.4452	0.8302	340.70	0.9453														
0.1824	365.35	0.4886	0.8671	339.97	0.9572														
0.2365	361.77	0.5759	0.9037	339.10	0.9681														
0.2834	359.33	0.6367	0.9528	337.78	0.9855														
0.3145	357.67	0.6720	1.0000	336.49	1.0000														
0.3442	356.16	0.7021																	
0.3734	354.80	0.7248																	
0.4014	353.55	0.7491																	
0.4303	352.32	0.7707																	
0.4581	351.12	0.7926																	
0.5224	348.77	0.8325																	
0.5879	346.51	0.8624																	

## AUXILIARY INFORMATION

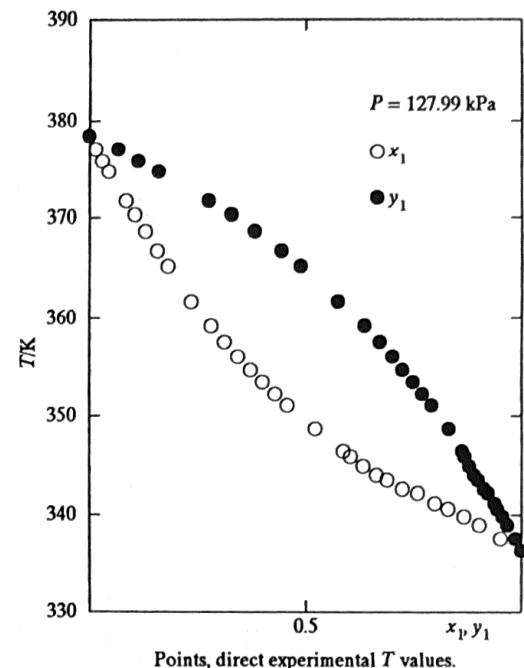
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of  $50 \text{ cm}^3$ , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum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

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at  $298.15 \text{ K}$  with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of  $\pm 0.02 \text{ kg m}^{-3}$ . A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition were  $\pm 0.002$  mole fraction for liquid phase and  $\pm 0.004$  mole fraction for vapor phase.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3590, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 927.07$ ; ref. 4.

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3949, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 802.29$ .

Errors:  $|\delta T|/K = 0.01$ ;  $|\delta P|/\text{Pa} = 10$ ;  $|\delta x_1| = 0.005$ ;  $|\delta y_1| = 0.01$ .



Points, direct experimental  $T$  values.

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
2. Ortega, J.; Hernández, P. Fluid Phase Equilib., 1996, 118, 249.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.
4. Ortega, J.; Peña, J. A. J. Chem. Eng. Jpn., 1994, 27, 351.

# SELECTED DATA ON MIXTURES

International DATA Series\*

3m. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

0147-1503/03/02-3328-40\$4.00

**Components:** 1. Methyl ethanone,  $C_3H_6O_2$  [79-20-9]  
2. 2-Butanol,  $C_4H_{10}O$  [78-92-2]

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

**Variables:**  $T$ , temperature

$x_i$ , mole fraction of component  $i$  in liquid phase

$y_i$ , mole fraction of component  $i$  in vapor phase

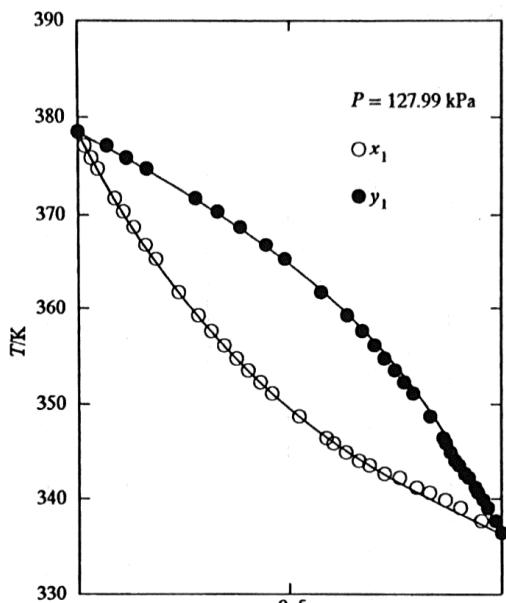
**Parameters:**  $P$ , pressure

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

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

	$P/kPa = 74.66$		$P/kPa = 101.32$		$P/kPa = 127.99$		
$x_1$	$T/K$	$y_1$	$T/K$	$y_1$	$T/K$	$y_1$	
0.00	364.04	0.0000	372.36	0.0000	378.56	0.0000	
0.05	358.27	0.2412	367.02	0.2178	374.49	0.1747	
0.10	353.36	0.4102	362.43	0.3760	370.72	0.3161	
0.15	349.18	0.5313	358.48	0.4932	367.25	0.4309	
0.20	345.61	0.6201	355.07	0.5817	364.05	0.5243	
0.25	342.54	0.6869	352.10	0.6501	361.11	0.6007	
0.30	339.89	0.7383	349.51	0.7041	358.42	0.6637	
0.40	335.54	0.8114	345.20	0.7833	353.68	0.7593	
0.50	332.14	0.8606	341.73	0.8387	349.68	0.8270	
0.60	329.39	0.8966	338.84	0.8805	346.30	0.8766	
0.70	327.06	0.9251	336.33	0.9145	343.41	0.9145	
0.75	326.01	0.9378	335.18	0.9296	342.12	0.9305	
0.80	325.00	0.9499	334.07	0.9441	340.91	0.9451	
0.85	324.03	0.9618	332.99	0.9581	339.76	0.9588	
0.90	323.06	0.9738	331.92	0.9719	338.66	0.9722	
0.95	322.10	0.9864	330.87	0.9858	337.58	0.9856	
1.00	321.12	1.0000	329.81	1.0000	336.49	1.0000	

Standard deviation  $\sigma(T)/K$ , relative standard deviation  $100\sigma(\delta P/P)$ , and absolute maximum deviation  $\delta_m(T)/K$  at  $P/kPa = 74.66$  are resp.: 0.125, 0.503, 0.389,  
at  $P/kPa = 101.32$  are resp.: 0.155, 0.597, 0.269,  
at  $P/kPa = 127.99$  are resp.: 0.230, 0.808, 0.543.



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

## AUXILIARY INFORMATION

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

**Computations:** The 31  $T_{exp}$  data at 74.66 kPa, 27  $T_{exp}$  data at 101.32 kPa and 31  $T_{exp}$  data at 127.99 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $\mu_i^E$ .

**Corrections:** Vapor pressure equation parameters were taken from ref. 4 and parameters  $A_i$  were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_y$ , ref. 5, and the molar volumes under saturation pressure  $V_i^0$ , ref. 6.

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

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table 3k: Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

## SOURCE OF DATA

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

$P/kPa$	$a_1/K$	$a_2/K^2$	$a_3/K$	$a_4/K^2$	
74.66	244.10 (12.0)	0 (0)	-14.401 (7.7)	0 (0)	
101.32	170.03 (18.5)	0 (0)	22.342 (14.7)	0 (0)	
127.99	356.16 (31.7)	0 (0)	-145.73 (15.0)	0 (0)	

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

$P/kPa$	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
74.66	14.26131	-2662.78	-53.46	15.21992	-3026.03	-86.60
101.32	14.25382	-2662.78	-53.46	15.20769	-3026.03	-86.60
127.99	14.26007	-2662.78	-53.46	15.21649	-3026.03	-86.60

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 81 and 82.
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. Tsionopoulos, 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

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

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0147-1503/3/302-84\$4.00

Components:	1. Ethyl ethanoate, $C_4H_8O_2$ [141-78-6] 2. 2-Butanol, $C_4H_{10}O$ [78-92-2]	Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Edited by: Skrzecz, A.; Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variables:	$T$ , temperature $x_i$ , mole fraction of component $i$ in liquid phase $y_i$ , mole fraction of component $i$ in vapor phase	SOURCE OF DATA
Parameters:	$P$ , pressure	Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2
Method:	Direct measurement of $T$ , $x_i$ and $y_i$ at constant $P$ ; ref. 1	

## DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$					
$x_1$	$T/K$	$y_1$	$x_1$	$T/K$	$y_1$
0.000	372.39	0.000	0.740	353.43	0.848
0.015	371.75	0.033	0.787	352.73	0.874
0.033	370.95	0.077	0.832	352.15	0.902
0.049	370.15	0.120	0.870	351.66	0.923
0.067	369.50	0.156	0.913	351.12	0.949
0.113	367.75	0.249	0.952	350.66	0.972
0.134	366.93	0.289	0.977	350.37	0.987
0.167	365.72	0.344	1.000	350.25	1.000
0.190	365.04	0.373			
0.220	364.08	0.420			
0.273	362.54	0.485			
0.372	359.90	0.592			
0.441	358.52	0.649			
0.472	357.93	0.672			
0.548	356.47	0.729			
0.592	355.75	0.757			
0.634	355.10	0.780			
0.666	354.54	0.801			
0.704	353.96	0.824			

## AUXILIARY INFORMATION

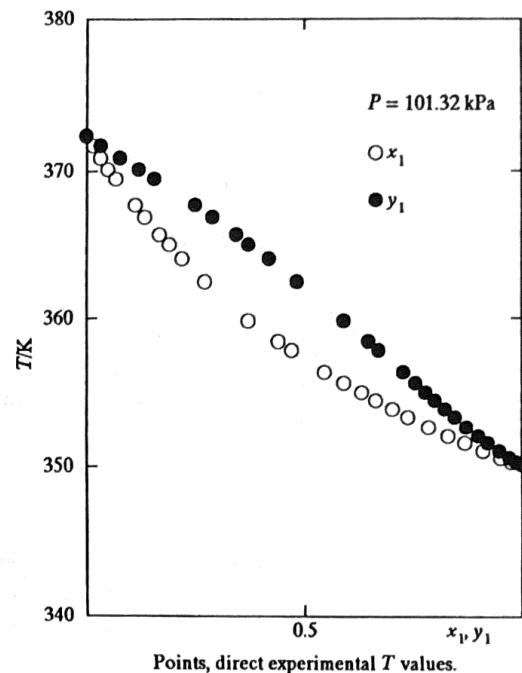
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a capacity of approx.  $60\text{ cm}^3$ , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a mercury manometer.

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

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15\text{ K}) = 1.3699, \rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 894.34$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15\text{ K}) = 1.3949, \rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 802.34$ .

Errors:  $|\delta T|/K = 0.01$ ;  $|\delta P|/\text{Pa} = 10$ ;  $|\delta x_1| = 0.003$ ;  $|\delta y_1| = 0.005$ .

Points, direct experimental  $T$  values.

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0147-1503(3)302-855\$4.00

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

**Variables:**  $T$ , temperature

$x_i$ , mole fraction of component  $i$  in liquid phase

$y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table 3k: Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

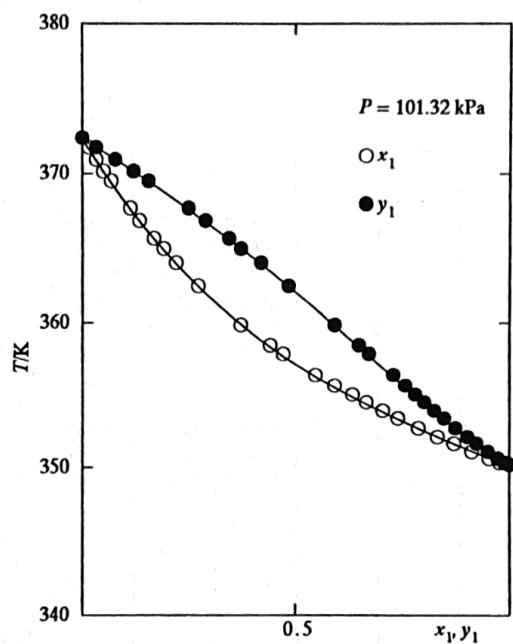
## SOURCE OF DATA

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

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

$x_1$	$T/K$	$y_1$				
0.00	372.39	0.0000				
0.05	370.19	0.1220				
0.10	368.18	0.2256				
0.15	366.36	0.3142				
0.20	364.70	0.3907				
0.25	363.19	0.4572				
0.30	361.81	0.5155				
0.40	359.38	0.6134				
0.50	357.32	0.6933				
0.60	355.55	0.7613				
0.70	354.00	0.8221				
0.75	353.29	0.8511				
0.80	352.62	0.8797				
0.85	351.99	0.9083				
0.90	351.38	0.9375				
0.95	350.80	0.9679				
1.00	350.25	1.0000				

Standard deviation  $\sigma(T)/K$ , relative standard deviation  $100\sigma(\delta P/P)$ , and absolute maximum deviation  $\delta_m(T)/K$  at  $P/kPa = 101.32$  are resp.: 0.063, 0.222, 0.122.



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

## AUXILIARY INFORMATION

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

**Computations:** The 27  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $\mu_i^E$ .

**Corrections:** Vapor pressure equation parameters were taken from ref. 4 and parameters  $A_i$  were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_{ij}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^0$ , ref. 6.

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

$P/kPa$	$a_1/K$	$a_2/K^2$	$a_3/K$	$a_4/K^2$	
101.32	175.41 (10.2)	0 (0)	-10.665 (7.8)	0 (0)	

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

$P/kPa$	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	14.12165	-2751.89	-60.68	15.20658	-3026.03	-86.60

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 84.
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. Tsionopoulos, C. AIChE J., 1974, 20, 263; 1975, 21, 827.
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## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3k. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

**Components:** 1. 2-Butanol, C<sub>4</sub>H<sub>10</sub>O /78-92-2/  
2. Methyl butanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> /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<sub>i</sub>, mole fraction of component i in liquid phase  
y<sub>i</sub>, mole fraction of component i in vapor phase  
**Parameters:** P, pressure  
**Method:** Direct measurement of T, x<sub>i</sub> and y<sub>i</sub> at constant P; ref. 1

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

## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

P/kPa = 74.66				P/kPa = 101.32							
x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>
0.0000	364.95	0.0000	0.7263	362.00	0.6884	0.0000	375.35	0.0000	0.6551	370.64	0.6453
0.0271	364.58	0.0503	0.7604	362.14	0.7168	0.0083	375.17	0.0136	0.6865	370.66	0.6706
0.0539	364.13	0.0902	0.7914	362.30	0.7464	0.0194	375.07	0.0304	0.7120	370.69	0.6926
0.0826	363.93	0.1283	0.8160	362.44	0.7748	0.0382	374.77	0.0594	0.7385	370.73	0.7160
0.1109	363.52	0.1700	0.8460	362.62	0.8043	0.0701	374.23	0.1096	0.7669	370.81	0.7417
0.1468	363.12	0.2207	0.8735	362.85	0.8365	0.1008	373.73	0.1542	0.7966	370.90	0.7689
0.1916	362.74	0.2638	0.8973	363.06	0.8650	0.1334	373.35	0.1940	0.8201	370.98	0.7921
0.2316	362.41	0.3085	0.9215	363.28	0.8958	0.1651	372.97	0.2316	0.8642	371.22	0.8385
0.2838	362.19	0.3506	0.9494	363.53	0.9293	0.1969	372.64	0.2651	0.8903	371.39	0.8658
0.3282	361.96	0.3933	0.9752	363.69	0.9641	0.2254	372.39	0.2936	0.9145	371.54	0.8935
0.3760	361.85	0.4308	0.9895	363.93	0.9825	0.2975	371.81	0.3608	0.9355	371.66	0.9158
0.4319	361.71	0.4728	1.0000	364.04	1.0000	0.3395	371.53	0.4008	0.9667	371.95	0.9549
0.4678	361.67	0.4999			0.3684	0.371.39	0.4218	0.9799	0.9722	372.13	0.9722
0.5050	361.66	0.5269			0.4572	0.370.88	0.4924	0.9929	0.9893	372.26	0.9893
0.5345	361.66	0.5432			0.5062	0.370.77	0.5268	1.0000	0.9999	372.36	1.0000
0.5787	361.69	0.5695			0.5380	0.370.70	0.5538				
0.6151	361.76	0.5924			0.5693	0.370.66	0.5761				
0.6394	361.78	0.6100			0.5995	0.370.63	0.5980				
0.6986	361.89	0.6609			0.6272	0.370.63	0.6216				

## AUXILIARY INFORMATION

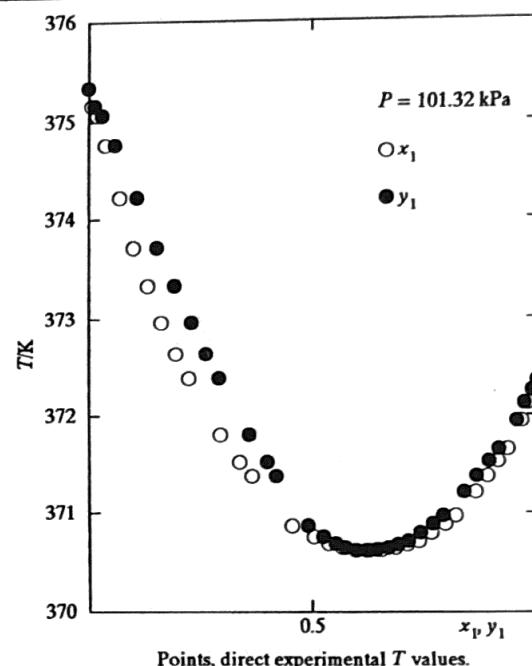
**Apparatus:** The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm<sup>3</sup>, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum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

**Procedure:** The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ± 0.02 kg·m<sup>-3</sup>. A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition were ± 0.002 mole fraction for liquid phase and ± 0.004 mole fraction for vapor phase.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3949, ρ(298.15 K)/kg·m<sup>-3</sup> = 802.29.

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3851, ρ(298.15 K)/kg·m<sup>-3</sup> = 892.37; ref. 4.

**Errors:** |δT|/K = 0.01; |δP|/Pa = 10; |δx<sub>1</sub>| = 0.003; |δy<sub>1</sub>| = 0.01.



## REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
- Ortega, J.; Hernández, P. Fluid Phase Equilib., 1996, 118, 249.
- Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.
- Ortega, J.; Susial, P. Ber. Bunsen-Ges. Phys. Chem., 1991, 95, 1214.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3k. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

0147-1503/02/3702-87\$4.00

**Components:** 1. 2-Butanol,  $C_4H_{10}O$  [78-92-2]  
 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  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

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

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

## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

 $P/kPa = 127.99$ 

$x_1$	$T/K$	$y_1$	$x_1$	$T/K$	$y_1$								
0.0000	382.54	0.0000	0.5882	377.71	0.5991								
0.0138	382.24	0.0220	0.6154	377.64	0.6240								
0.0308	381.93	0.0478	0.6490	377.60	0.6482								
0.0529	381.66	0.0795	0.6673	377.59	0.6629								
0.1106	380.83	0.1596	0.6917	377.58	0.6854								
0.1460	380.55	0.2061	0.7182	377.59	0.7073								
0.1780	379.95	0.2441	0.7407	377.60	0.7290								
0.2035	379.71	0.2723	0.7664	377.62	0.7532								
0.2191	379.64	0.2918	0.7925	377.69	0.7771								
0.2542	379.34	0.3232	0.8441	377.82	0.8256								
0.2804	379.12	0.3510	0.8809	377.95	0.8625								
0.3144	378.88	0.3822	0.9109	378.06	0.8935								
0.3805	378.41	0.4409	0.9360	378.19	0.9225								
0.4179	378.33	0.4608	0.9566	378.29	0.9448								
0.4468	378.13	0.4817	0.9858	378.47	0.9817								
0.4669	378.09	0.5053	1.0000	378.56	1.0000								
0.4990	377.97	0.5298											
0.5276	377.87	0.5532											
0.5550	377.77	0.5763											

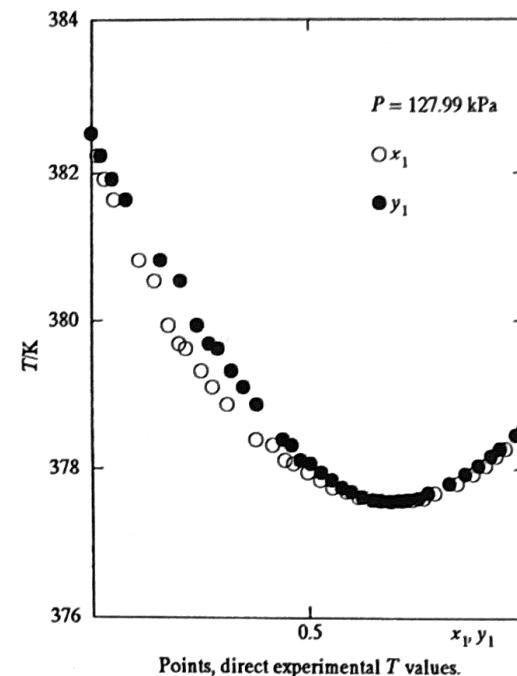
## AUXILIARY INFORMATION

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

**Procedure:** The procedure was described in ref. 3. The compositions were determined by measuring their densities at  $298.15\text{ K}$  with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of  $\pm 0.02\text{ kg}\cdot\text{m}^{-3}$ . A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition were  $\pm 0.002$  mole fraction for liquid phase and  $\pm 0.004$  mole fraction for vapor phase.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15\text{ K}) = 1.3949, \rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 802.29$ .  
 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15\text{ K}) = 1.3851, \rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3} = 892.37$ ; ref. 4.

**Errors:**  $|\delta T|/K = 0.01$ ;  $|\delta P|/\text{Pa} = 10$ ;  $|\delta x_1| = 0.003$ ;  $|\delta y_1| = 0.01$ .

Points, direct experimental  $T$  values.

## REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
- Ortega, J.; Hernández, P. Fluid Phase Equilib., 1996, 118, 249.
- Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.
- Ortega, J.; Susial, P. Ber. Bunsen-Ges. Phys. Chem., 1991, 95, 1214.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3m. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

0107-1503(2003)30:2;88-94;00

**Components:** 1. 2-Butanol,  $C_4H_{10}O$  /78-92-2/  
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  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase  
**Parameters:**  $P$ , pressure  
**Method:** Calculation from direct experimental liquid-vapor equilibrium temperature,  $T_{exp}$ , data at variable  $x_i$  and constant  $P$ ; ref. 1

**Author(s)** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table 3k; Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

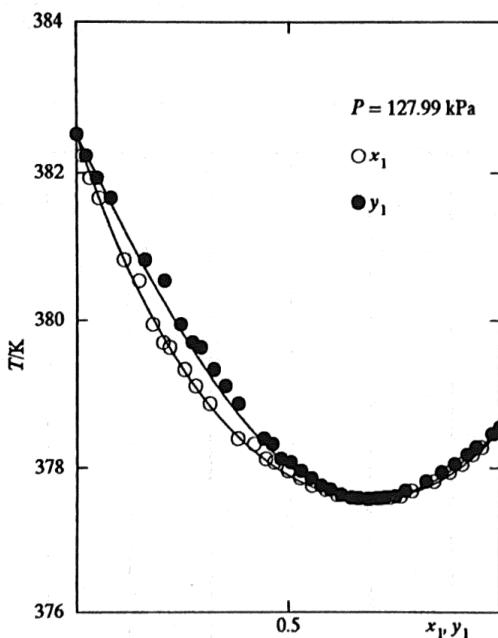
## SOURCE OF DATA

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

Notes: The table reports smoothed values of  $T$  and calculated values of  $y_1$

$x_1$	$P/kPa = 74.66$		$P/kPa = 101.32$		$P/kPa = 127.99$		
	$T/K$	$y_1$	$T/K$	$y_1$	$T/K$	$y_1$	
0.00	364.95	0.0000	375.35	0.0000	382.54	0.0000	
0.05	364.20	0.0712	374.51	0.0726	381.71	0.0711	
0.10	363.60	0.1345	373.78	0.1384	380.99	0.1359	
0.15	363.10	0.1917	373.15	0.1986	380.37	0.1956	
0.20	362.70	0.2441	372.62	0.2542	379.83	0.2512	
0.25	362.37	0.2926	372.16	0.3059	379.37	0.3032	
0.30	362.12	0.3383	371.77	0.3545	378.97	0.3524	
0.40	361.78	0.4235	371.19	0.4443	378.35	0.4443	
0.50	361.65	0.5045	370.81	0.5275	377.92	0.5306	
0.60	361.70	0.5853	370.64	0.6078	377.68	0.6145	
0.70	361.93	0.6698	370.66	0.6889	377.60	0.6992	
0.75	362.12	0.7148	370.75	0.7312	377.63	0.7430	
0.80	362.36	0.7626	370.90	0.7757	377.71	0.7884	
0.85	362.67	0.8140	371.12	0.8234	377.83	0.8360	
0.90	363.04	0.8699	371.43	0.8754	378.01	0.8865	
0.95	363.49	0.9314	371.83	0.9335	378.25	0.9409	
1.00	364.04	1.0000	372.36	1.0000	378.56	1.0000	

Standard deviation  $\sigma(T)/K$ , relative standard deviation  $100\sigma(\delta P/P)$ , and absolute maximum deviation  $\delta_m(T)/K$  at  $P/kPa = 74.66$  are resp.: 0.040, 0.144, 0.132,  
at  $P/kPa = 101.32$  are resp.: 0.029, 0.097, 0.066,  
at  $P/kPa = 127.99$  are resp.: 0.043, 0.135, 0.131.



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

## AUXILIARY INFORMATION

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

Computations: The 31  $T_{exp}$  data at 74.66 kPa, 34  $T_{exp}$  data at 101.32 kPa and 35  $T_{exp}$  data at 127.99 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $\mu_i^E$ .

Corrections: Vapor pressure equation parameters were taken from ref. 4 and parameters  $A_i$  were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted [for in terms of the 2nd molar virial coefficients  $[i]B_y$ , ref. 5, and the molar volumes under saturation pressure  $V_i^0$ , ref. 6].

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

$P/kPa$	$a_1/K$	$a_2/K^2$	$a_3/K$	$a_4/K^2$	
74.66	97.292 (7.4)	0 (0)	58.187 (7.1)	0 (0)	
101.32	210.45 (5.5)	0 (0)	-36.641 (3.9)	0 (0)	
127.99	135.93 (9.2)	0 (0)	-6.698 (7.6)	0 (0)	

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

$P/kPa$	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
74.66	15.21992	-3026.03	-86.60	14.10098	-2926.72	-65.94
101.32	15.20769	-3026.03	-86.60	14.07732	-2926.72	-65.94
127.99	15.21649	-3026.03	-86.60	14.09617	-2926.72	-65.94

## REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
- Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 86 and 87.
- Wilson, G. M. J. Am. Chem. Soc., 1964, 86, 127.
- 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.
- Tsonopoulos, C. AICHE J., 1974, 20, 263; 1975, 21, 827.
- Yen, L. C.; Woods, S. S. AICHE J., 1966, 12, 95.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3k LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

National Institute of Standards and Technology, Boulder, CO 80305-3320

0147-1503/02/7002-8984\$00

Components:	1. 2-Butanol, C <sub>4</sub> H <sub>10</sub> O /78-92-2/ 2. Ethyl propanoate, C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> /105-37-3/	Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Edited by: Skrzecz, A.; Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variables:	T, temperature $x_i$ , mole fraction of component <i>i</i> in liquid phase $y_i$ , mole fraction of component <i>i</i> in vapor phase	
Parameters:	P, pressure	
Method:	Direct measurement of T, $x_i$ and $y_i$ at constant P; ref. 1	SOURCE OF DATA Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES											
P/kPa = 101.32											
$x_1$	T/K	$y_1$	$x_1$	T/K	$y_1$						
0.000	371.92	0.000	0.692	369.96	0.649						
0.033	371.10	0.037	0.791	370.70	0.751						
0.069	370.80	0.079	0.849	371.15	0.814						
0.105	370.47	0.118	0.861	371.25	0.828						
0.180	369.87	0.196	0.877	371.38	0.846						
0.196	369.77	0.213	0.910	371.65	0.884						
0.239	369.63	0.253	0.931	371.85	0.910						
0.284	369.49	0.295	0.949	372.02	0.934						
0.321	369.40	0.328	0.971	372.18	0.961						
0.368	369.33	0.370	0.985	372.29	0.979						
0.400	369.33	0.395	1.000	372.39	1.000						
0.424	369.33	0.417									
0.445	369.34	0.435									
0.463	369.37	0.450									
0.497	369.39	0.477									
0.538	369.45	0.510									
0.576	369.53	0.541									
0.606	369.62	0.569									
0.650	369.76	0.610									

## AUXILIARY INFORMATION

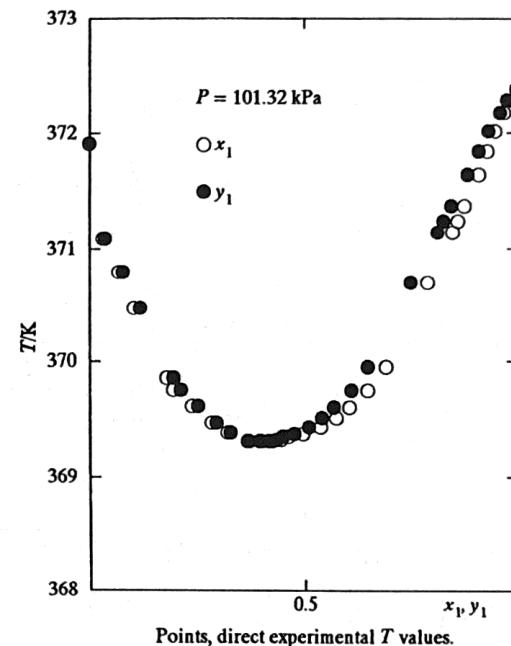
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a capacity of approx. 60 cm<sup>3</sup>, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätbau Wertheim) and measured with a mercury manometer.

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

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3949, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 802.34$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3811, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 883.93$ .

Errors:  $|\delta T|/K = 0.05$ ;  $|\delta P|/\text{Pa} = 10$ ;  $|8x_1| = 0.005$ ;  $|8y_1| = 0.01$ .



Points, direct experimental T values.

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
2. Hernández, P.; Ortega, J. J. Chem. Eng. Data, 1997, 42, 1090.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3m. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

0147-1503/02-954-00

**Components:** 1. 2-Butanol,  $C_4H_{10}O$  [78-92-2]  
 2. Ethyl propanoate,  $C_5H_{10}O_2$  [105-37-3]

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

**Variables:**  $T$ , temperature

$x_i$ , mole fraction of component  $i$  in liquid phase

$y_i$ , mole fraction of component  $i$  in vapor phase

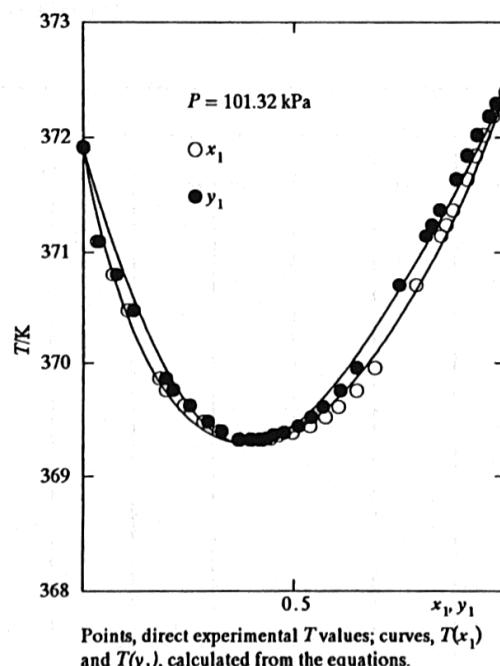
**Parameters:**  $P$ , pressure

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

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

	$P/kPa = 101.32$					
$x_1$	$T/K$	$y_1$				
0.00	371.92	0.0000				
0.05	371.07	0.0717				
0.10	370.47	0.1316				
0.15	370.04	0.1838				
0.20	369.74	0.2311				
0.25	369.53	0.2751				
0.30	369.39	0.3170				
0.40	369.30	0.3984				
0.50	369.41	0.4801				
0.60	369.69	0.5658				
0.70	370.14	0.6582				
0.75	370.41	0.7077				
0.80	370.73	0.7597				
0.85	371.09	0.8146				
0.90	371.48	0.8728				
0.95	371.92	0.9345				
1.00	372.39	1.0000				

Standard deviation  $\sigma(T)/K$ , relative standard deviation  $100\sigma(\delta P/P)$ , and absolute maximum deviation  $\delta_m(T)/K$  at  $P/kPa = 101.32$  are resp.: 0.079, 0.272, 0.216.



## AUXILIARY INFORMATION

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

**Computations:** The 30  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $\mu_i^E$ .

**Corrections:** Vapor pressure equation parameters were taken from ref. 4 and parameters  $A_i$  were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_i$ , ref. 5, and the molar volumes under saturation pressure  $V_i^0$ , ref. 6.

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

$P/kPa$	$a_1/K$	$a_2/K^2$	$a_3/K$	$a_4/K^2$	
101.32	-84.410 (10.2)	0 (0)	279.33 (17.3)	0 (0)	

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

$P/kPa$	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	15.20658	-3026.03	-86.60	14.15498	-2935.11	-64.15

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 89.
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. 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

Compiled by Thermodynamics Research Center

National Institute of Standards and Technology, Boulder, CO 80303-3328

0147-1503/02/3002-91\$4.00

Components:	1. 2-Butanol, C <sub>4</sub> H <sub>10</sub> O /78-92-2/ 2. Propyl ethanoate, C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> /109-60-4/	Author(s) of table:	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Edited by:	Skrzecz, A.; Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variables:	T, temperature		
x <sub>i</sub> , mole fraction of component i in liquid phase			
y <sub>i</sub> , mole fraction of component i in vapor phase			
Parameters:	P, pressure		
Method:	Direct measurement of T, x <sub>i</sub> and y <sub>i</sub> at constant P; ref. 1		

## SOURCE OF DATA

González, C.; Ortega, J.; Hernández, P.; Galván, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32

x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>
0.0000	374.31	0.0000	0.6370	370.76	0.6270
0.0450	373.55	0.0630	0.6390	370.77	0.6300
0.0920	373.05	0.1190	0.6700	370.78	0.6540
0.1350	372.64	0.1690	0.7000	370.79	0.6810
0.1790	372.26	0.2180	0.7320	370.85	0.7090
0.2200	371.96	0.2590	0.7650	370.92	0.7400
0.2580	371.72	0.2960	0.7980	371.01	0.7710
0.3030	371.48	0.3380	0.8310	371.14	0.8040
0.3460	371.26	0.3780	0.8660	371.25	0.8400
0.3890	371.10	0.4180	0.9010	371.42	0.8770
0.4260	370.96	0.4500	0.9330	371.62	0.9140
0.4620	370.88	0.4800	0.9670	371.88	0.9530
0.4950	370.84	0.5080	0.9830	371.98	0.9730
0.5230	370.80	0.5310	1.0000	372.27	1.0000
0.5290	370.77	0.5370			
0.5580	370.75	0.5620			
0.5770	370.75	0.5760			
0.5860	370.76	0.5850			
0.6050	370.76	0.5980			

## AUXILIARY INFORMATION

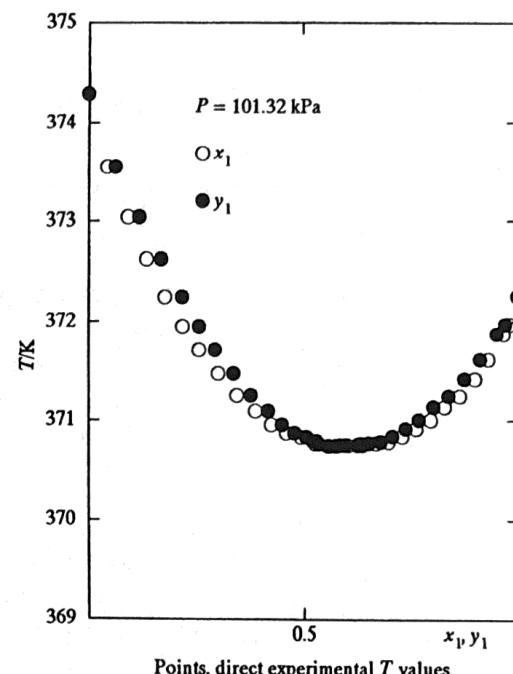
**Apparatus:** The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm<sup>3</sup>, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and a Desgranges et Huot model PPC2 pressure controller/calibrator with an uncertainty of  $\pm 0.02$  kPa. The temperatures were measured by a digital thermometer Comark Electronics model 6800 with a PT-100 sensor. The thermometer was periodically calibrated with respect to the ITS-90 using a standard ASL-F25 thermometer with the estimated uncertainty of the reading 0.02 %.

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

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc; n(D, 298.15 K) = 1.3949,  $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3}$  = 802.58.

2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc; n(D, 298.15 K) = 1.3816,  $\rho(298.15\text{ K})/\text{kg}\cdot\text{m}^{-3}$  = 882.67.

**Errors:** | $\delta T$ |/K = 0.02; | $\delta P$ |/Pa = 10; | $\delta x_1$ | = 0.005; | $\delta y_1$ | = 0.01.



Points, direct experimental T values.

## REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
- González, C.; Ortega, J.; Hernández, P.; Galván, S. J. Chem. Eng. Data, 1999, 44, 772.
- Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3m. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

047-1503/02-924-00

**Components:** 1. 2-Butanol, C<sub>4</sub>H<sub>10</sub>O [78-92-2]  
2. Propyl ethanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> [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<sub>i</sub>, mole fraction of component i in liquid phase

y<sub>i</sub>, mole fraction of component i in vapor phase

**Parameters:** P, pressure

**Method:** Calculation from direct experimental liquid-vapor equilibrium temperature, T<sub>exp</sub>, data at variable x<sub>i</sub> and constant P; ref. 1

**Author(s)** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table 3k: Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

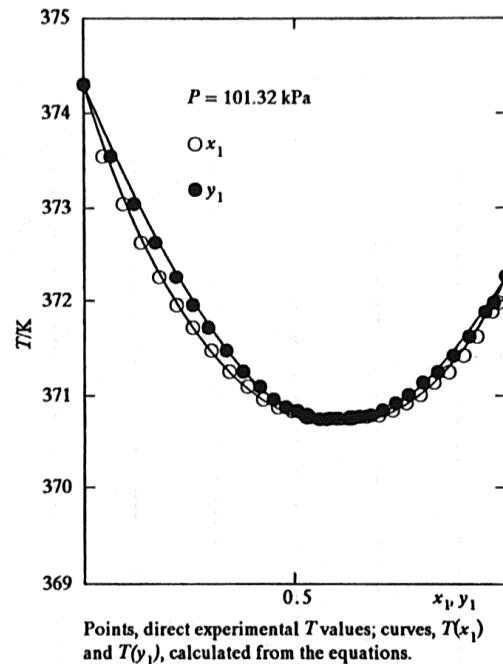
## SOURCE OF DATA

González, C.; Ortega, J.; Hernández, P.; Galván, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); FIRST PUBLISHED RESULTS

Notes: The table reports smoothed values of T and calculated values of y<sub>i</sub>

x <sub>i</sub>	T/K	y <sub>i</sub>				
0.00	374.31	0.0000				
0.05	373.64	0.0680				
0.10	373.06	0.1303				
0.15	372.56	0.1881				
0.20	372.14	0.2420				
0.25	371.79	0.2927				
0.30	371.49	0.3408				
0.40	371.05	0.4312				
0.50	370.80	0.5168				
0.60	370.71	0.6007				
0.70	370.79	0.6863				
0.75	370.89	0.7309				
0.80	371.04	0.7775				
0.85	371.25	0.8267				
0.90	371.52	0.8795				
0.95	371.85	0.9368				
1.00	372.27	1.0000				

Standard deviation σ(T)/K, relative standard deviation 100σ(ΔP/P), and absolute maximum deviation δ<sub>m</sub>(T)/K at P/kPa = 101.32 are resp.: 0.060, 0.209, 0.132.



Points, direct experimental T values; curves, T(x<sub>i</sub>) and T(y<sub>i</sub>), calculated from the equations.

## AUXILIARY INFORMATION

**Measurements:** The T<sub>exp</sub> data at 101.32 kPa are reported in ref. 2.

**Computations:** The 33 T<sub>exp</sub> data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies μ<sub>i</sub><sup>E</sup>.

**Corrections:** Vapor pressure equation parameters were taken from ref. 4 and parameters A<sub>i</sub> were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients B<sub>ij</sub>, ref. 5, and the molar volumes under saturation pressure V<sub>i</sub><sup>0</sup>, ref. 6.

**Errors:** Standard deviation σ(T) = [Σ(T-T<sub>exp</sub>)<sup>2</sup>/(N-n-2)]<sup>1/2</sup>,  
Relative standard deviation 100σ(ΔP/P) = 100[Σ((P-P<sub>exp</sub>)/P<sub>exp</sub>)<sup>2</sup>/(N-n-2)]<sup>1/2</sup>,  
N, number of experimental points, ref. 2,  
n, number of coefficients in the smoothing equation.

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

P/kPa	a <sub>1</sub> /K	a <sub>2</sub> /K <sup>2</sup>	a <sub>3</sub> /K	a <sub>4</sub> /K <sup>2</sup>	
101.32	143.04 (14.5)	0 (0)	-8.726 (11.8)	0 (0)	

The standard deviations σ(a<sub>i</sub>) of the coefficients a<sub>i</sub> are given in parentheses.

P/kPa	A <sub>1</sub>	B <sub>1</sub>	C <sub>1</sub>	A <sub>2</sub>	B <sub>2</sub>	C <sub>2</sub>
101.32	15.21103	-3026.03	-86.60	13.95351	-2840.15	-70.07

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 91.
3. Wilson, G. M. J. Am. Chem. Soc., 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1965, k-5010, 1969, k-5550, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
5. Tsionopoulos, 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

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

Compiled by Thermodynamics Research Center

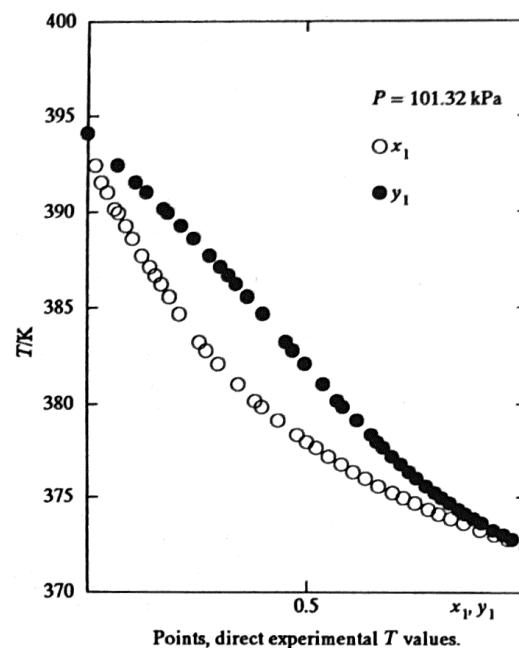
Components:	1. 2-Butanol, C <sub>4</sub> H <sub>10</sub> O [78-92-2] 2. Ethyl butanoate, C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> [105-54-4]	Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Edited by: Skrzecz, A.; Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variables:	T, temperature	
	x <sub>i</sub> , mole fraction of component i in liquid phase	
Parameters:	y <sub>i</sub> , mole fraction of component i in vapor phase	SOURCE OF DATA
Method:	P, pressure	Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

P/kPa = 101.32									
x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>	
0.000	394.18	0.000	0.401	379.90	0.584	0.958	372.83	0.968	
0.018	392.53	0.069	0.439	379.15	0.617	1.000	372.39	1.000	
0.032	391.62	0.110	0.482	378.37	0.649				
0.046	391.12	0.135	0.503	378.01	0.662				
0.063	390.22	0.175	0.524	377.70	0.676				
0.072	390.02	0.185	0.552	377.21	0.695				
0.089	389.32	0.215	0.582	376.78	0.715				
0.104	388.65	0.245	0.607	376.38	0.734				
0.126	387.75	0.282	0.635	376.04	0.751				
0.144	387.17	0.306	0.665	375.63	0.772				
0.157	386.70	0.325	0.697	375.27	0.793				
0.170	386.27	0.341	0.722	375.01	0.808				
0.189	385.63	0.367	0.747	374.72	0.826				
0.213	384.72	0.403	0.778	374.40	0.846				
0.259	383.28	0.455	0.801	374.16	0.862				
0.274	382.85	0.471	0.829	373.91	0.880				
0.302	382.15	0.499	0.858	373.66	0.899				
0.348	381.10	0.540	0.895	373.31	0.925				
0.386	380.20	0.572	0.927	373.06	0.947				

## AUXILIARY INFORMATION

Apparatus:	The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a capacity of approx. 60 cm <sup>3</sup> , ref. 3.
	Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a mercury manometer.
Procedure:	The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of $\pm 0.02 \text{ kg m}^{-3}$ . A polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition < 0.002 mole fraction.
Materials:	1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3949, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 802.34$ . 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3898, \rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.94$ .
Errors:	$\delta T$  /K = 0.02;   $\delta P$  /Pa = 10;   $\delta x_1$   = 0.005;   $\delta y_1$   = 0.01.



## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3h, 1994, 22(4).
2. Hernández, P.; Ortega, J. J. Chem. Eng. Data, 1997, 42, 1090.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. J. Chem. Eng. Data, 1986, 31, 339.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3m. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80303-3328

Compiled by Thermodynamics Research Center

0147-1503/03/0502-04\$4.00/0

**Components:** 1. 2-Butanol, C<sub>4</sub>H<sub>10</sub>O /78-92-2/  
2. Ethyl butanoate, C<sub>6</sub>H<sub>12</sub>O<sub>2</sub> /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<sub>i</sub>, mole fraction of component i in liquid phase

y<sub>i</sub>, mole fraction of component i in vapor phase

**Parameters:** P, pressure

**Method:** Calculation from direct experimental liquid-vapor equilibrium temperature, T<sub>exp</sub>, data at variable x<sub>i</sub> and constant P; ref. 1

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table 3k: Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

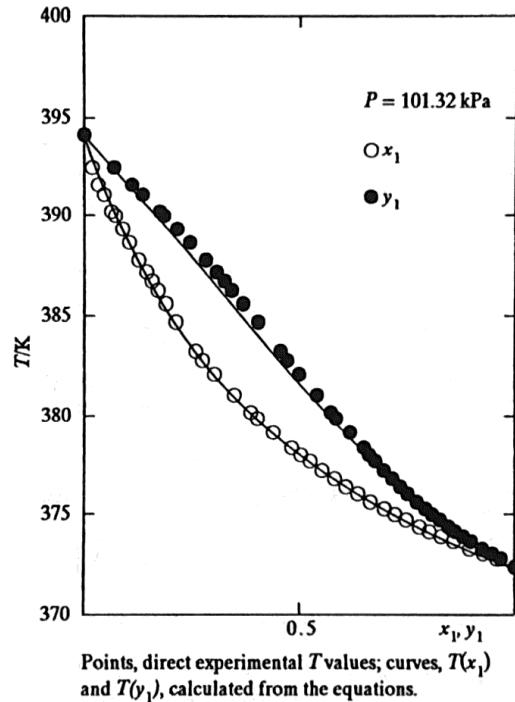
## SOURCE OF DATA

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

Notes: The table reports smoothed values of T and calculated values of y<sub>i</sub>

x <sub>i</sub>	T/K	y <sub>i</sub>				
0.00	394.18	0.0000				
0.05	391.26	0.1181				
0.10	388.84	0.2146				
0.15	386.80	0.2956				
0.20	385.04	0.3653				
0.25	383.52	0.4264				
0.30	382.17	0.4807				
0.40	379.92	0.5749				
0.50	378.09	0.6557				
0.60	376.56	0.7283				
0.70	375.28	0.7964				
0.75	374.70	0.8296				
0.80	374.17	0.8627				
0.85	373.68	0.8960				
0.90	373.22	0.9297				
0.95	372.79	0.9643				
1.00	372.39	1.0000				

Standard deviation σ(T)/K, relative standard deviation 100σ(ΔP/P), and absolute maximum deviation δ<sub>m</sub>(T)/K at P/kPa = 101.32 are resp.: 0.171, 0.480, 0.592.



Points, direct experimental T values; curves, T(x<sub>i</sub>) and T(y<sub>i</sub>), calculated from the equations.

## AUXILIARY INFORMATION

**Measurements:** The T<sub>exp</sub> data at 101.32 kPa are reported in ref. 2.

**Computations:** The 40 T<sub>exp</sub> data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies μ<sub>i</sub><sup>E</sup>.

**Corrections:** Vapor pressure equation parameters were taken from ref. 4 and parameters A<sub>i</sub> were modified according to the experimental boiling points of pure substances. Vapor-phase imperfection and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients B<sub>ij</sub>, ref. 5, and the molar volumes under saturation pressure V<sub>i</sub><sup>0</sup>, ref. 6.

**Errors:** Standard deviation σ(T) = [Σ(T - T<sub>exp</sub>)<sup>2</sup>/(N-n-2)]<sup>1/2</sup>,  
Relative standard deviation 100σ(ΔP/P) = 100[Σ((P - P<sub>exp</sub>)/P<sub>exp</sub>)<sup>2</sup>/(N-n-2)]<sup>1/2</sup>,  
N, number of experimental points, ref. 2,  
n, number of coefficients in the smoothing equation.

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

P/kPa	a <sub>1</sub> /K	a <sub>2</sub> /K <sup>2</sup>	a <sub>3</sub> /K	a <sub>4</sub> /K <sup>2</sup>	
101.32	87.881 (25.8)	0 (0)	25.121 (23.7)	0 (0)	

The standard deviations σ(a<sub>i</sub>) of the coefficients a<sub>i</sub> are given in parentheses.

P/kPa	A <sub>1</sub>	B <sub>1</sub>	C <sub>1</sub>	A <sub>2</sub>	B <sub>2</sub>	C <sub>2</sub>
101.32	15.20658	-3026.03	-86.60	12.15878	-2121.97	-112.77

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A, 2003, 31, 93.
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. Tsionopoulos, 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\*

## 2c. EXCESS VOLUME

Compiled by Thermodynamics Research Center

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

0147-1503/02/3302-95\$4.00

**Components:** 1. Methyl ethanoate,  $C_3H_6O_2$  [79-20-9]  
 2. 2-Butanol,  $C_4H_{10}O$  [78-92-2]

**State:** Binary system, single-phase liquid; pure components, both liquid

**Variables:**  $V^E$ , molar excess volume

$x_i$ , mole fraction of component  $i$

**Parameters:**  $T$ , temperature

**Constants:**  $P$ , pressure

**Method:** Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_i$ ; ref. 1

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

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

## SOURCE OF DATA

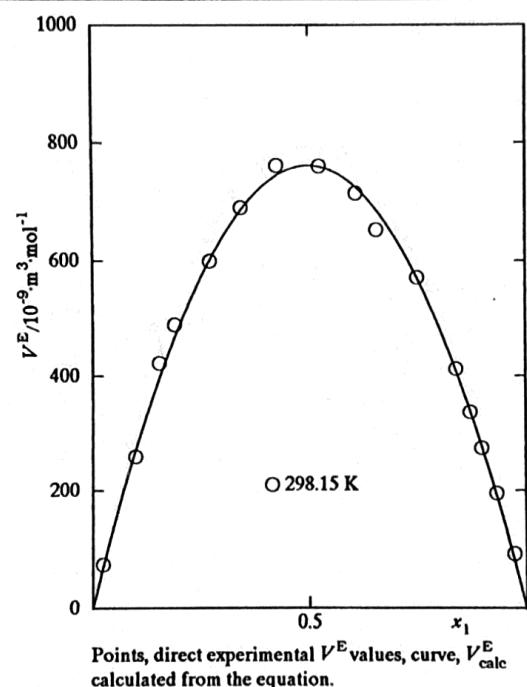
Ortega, J.; Hernández, P. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

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

T/K = 298.15

$x_1$	$V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$
0.0238	74.6
0.0984	260.0
0.1532	423.9
0.1890	490.0
0.2704	599.3
0.3426	691.5
0.4259	762.4
0.5249	760.7
0.6099	715.5
0.6565	652.9
0.7512	571.0
0.8405	413.6
0.8728	337.2
0.8992	275.0
0.9323	195.9
0.9729	92.8



## AUXILIARY INFORMATION

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

**Procedure:** The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed  $2.5 \text{ cm}^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $n(D, 298.15 \text{ K}) = 1.3590$ , ref. 4,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 926.97$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 329.81$ .  
 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $n(D, 298.15 \text{ K}) = 1.3949$ ,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 802.29$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 372.36$ .

**Errors:**  $\delta T/\text{K} = 0.02$ ;  $\delta x_1 = 0.0005$ ;  $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} < 10$ .

## SMOOTHING EQUATION

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

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_d$ , and maximum deviation  $\delta_m$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_d$	$\delta_m$
	$10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$						
298.15	3054 (22)					14.7	35.7

The standard deviations  $\sigma a_i$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$ ;  $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
 All direct experimental values equally weighted

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
2. Ortega, J.; Hernández, P. Fluid Phase Equilib., 1996, 118, 249.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. J. Chem. Thermodyn., 1985, 17, 1127.
4. Ortega, J.; Peña, J. A. J. Chem. Eng. Jpn., 1994, 27, 351.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 2c. EXCESS VOLUME

Compiled by Thermodynamics Research Center

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

0147-1503/3/302-665\$4.00

**Components:** 1. Ethyl ethanone,  $C_4H_8O_2$  /141-78-6/  
2. 2-Butanol,  $C_4H_{10}O$  /78-92-2/

**State:** Binary system, single-phase liquid; pure components, both liquid**Variables:**  $V^E$ , molar excess volume $x_i$ , mole fraction of component  $i$ **Parameters:**  $T$ , temperature**Constants:**  $P$ , pressure**Method:** Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_i$ ; ref. 1

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

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

## SOURCE OF DATA

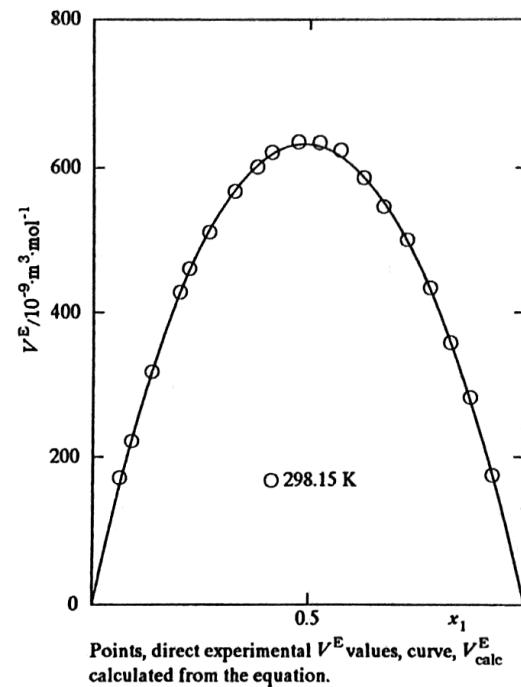
Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

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

T/K = 298.15

$x_1$	$V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$
0.0617	172
0.0888	223
0.1354	320
0.2003	428
0.2222	460
0.2671	512
0.3264	568
0.3784	601
0.4120	621
0.4745	634
0.5228	633
0.5730	623
0.6254	587
0.6729	547
0.7273	501
0.7809	434
0.8286	360
0.8757	285
0.9257	176



## SMOOTHING EQUATION

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

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_d$ , and maximum deviation  $\delta_m$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_d$	$\delta_m$
	$10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$						
298.15	2528.9 (6.9)	-113.7 (13.5)	225 (31)			4.2	9.8

The standard deviations  $\sigma(a_i)$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$ ;  $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
 All direct experimental values equally weighted

## AUXILIARY INFORMATION

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

**Procedure:** The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed  $2.5 \text{ cm}^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3699$ ,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 894.34$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 350.25$ .  
 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3949$ ,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 802.34$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 372.39$ .

**Errors:**  $\delta T/\text{K} = 0.02$ ;  $\delta x_1 = 0.0005$ ;  $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} < 8$ .

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
2. Hernández, P.; Ortega, J. J. Chem. Eng. Data, 1997, 42, 1090.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. J. Chem. Thermodyn., 1985, 17, 1127.

## SELECTED DATA ON MIXTURES

## International DATA Series\*

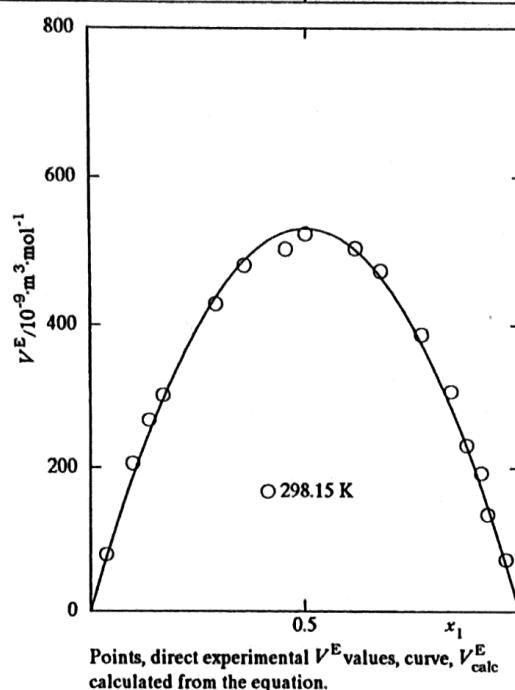
## 2c. EXCESS VOLUME

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

Compiled by Thermodynamics Research Center

Components:	1. 2-Butanol, C <sub>4</sub> H <sub>10</sub> O /78-92-2/ 2. Methyl butanoate, C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> /623-42-7/	Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State:	Binary system, single-phase liquid; pure components, both liquid	Edited by: Skrzecz, A.; Mączyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
Variables:	V <sup>E</sup> , molar excess volume	
Parameters:	x <sub>i</sub> , mole fraction of component i	
Constants:	T, temperature	
Method:	P, pressure	
	Calculation of V <sup>E</sup> from density measurements at constant T and P and variable x <sub>i</sub> ; ref. 1	SOURCE OF DATA Ortega, J.; Hernández, P. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES	
Notes: P = 101.32 kPa.	
T/K = 298.15	
x <sub>i</sub>	V <sup>E</sup> /10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>
0.0364	79.5
0.0985	206.9
0.1376	268.6
0.1691	304.3
0.2928	429.5
0.3586	480.1
0.4542	502.8
0.4999	522.5
0.6158	503.0
0.6732	473.3
0.7694	387.7
0.8380	309.8
0.8751	232.9
0.9089	194.3
0.9244	136.5
0.9672	73.5



AUXILIARY INFORMATION							
Apparatus: The density was determined by an Anton Paar Model DMA-55 vibrating-tube digital densimeter with a precision of $\pm 0.02 \text{ kg}\cdot\text{m}^{-3}$ . The temperature was controlled at $\pm 0.01 \text{ K}$ with a Heto ultrathermostat.							
Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm <sup>3</sup> glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.							
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3949, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3}$ = 802.29, $T_b(101.32 \text{ kPa})/\text{K}$ = 372.36. 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; n(D, 298.15 K) = 1.3851, ref. 4, $\rho(298.15 \text{ K})/\text{kg}\cdot\text{m}^{-3}$ = 892.35, $T_b(101.32 \text{ kPa})/\text{K}$ = 375.35.							
Errors: $\delta T/\text{K} = 0.02$ ; $\delta x_i = 0.0005$ ; $\delta V^E/10^{-9} \cdot \text{m}^3 \cdot \text{mol}^{-1} < 10$ .							

SMOOTHING EQUATION							
$V^E_{\text{calc}} = x_1 x_2 \sum_{i=1}^n a_i (x_1 - x_2)^{i-1}$							
Coefficients $a_i$ in the smoothing equation, standard deviation $\sigma_d$ , and maximum deviation $\delta_m$ determined by least-squares analysis.							
T/K	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	$\sigma_d$	$\delta_m$
298.15	2123.4 (19.9)					13.2	23.6

The standard deviations  $\sigma(a_i)$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$ ;  $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
All direct experimental values equally weighted

- #### REFERENCES
- Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
  - Ortega, J.; Hernández, P. *Fluid Phase Equilib.*, 1996, 118, 249.
  - Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. *J. Chem. Thermodyn.*, 1985, 17, 1127.
  - Ortega, J.; Susial, P. *Ber. Bunsen-Ges. Phys. Chem.*, 1991, 95, 1214.

**SELECTED DATA ON MIXTURES**  
International DATA Series\*

2c. EXCESS VOLUME

Compiled by Thermodynamics Research Center

Components: 1. 2-Butanol, C<sub>4</sub>H<sub>10</sub>O /78-92-2/  
2. Ethyl propanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> /105-37-3/  
State: Binary system, single-phase liquid; pure components, both liquid  
Variables: V<sup>E</sup>, molar excess volume  
x<sub>i</sub>, mole fraction of component i  
Parameters: T, temperature  
Constants: P, pressure  
Method: Calculation of V<sup>E</sup> from density measurements at constant T and P and variable x<sub>i</sub>; ref. 1

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

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

SOURCE OF DATA

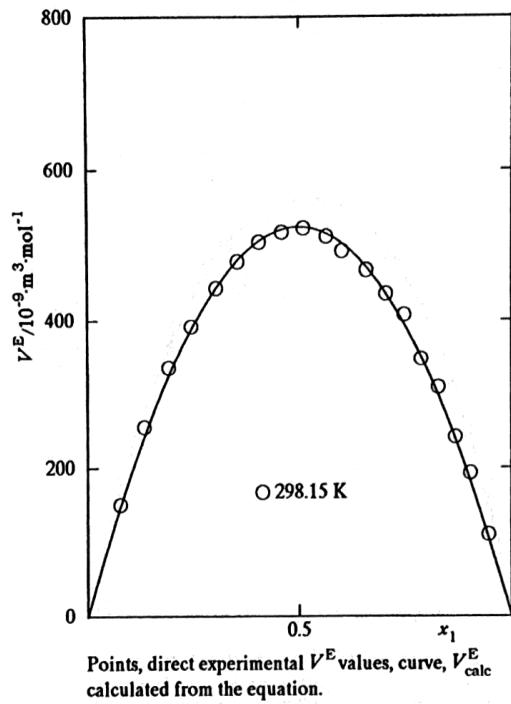
Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: P = 101.32 kPa.

T/K = 298.15

x <sub>1</sub>	V <sup>E</sup> /10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>
0.0766	152
0.1343	256
0.1928	336
0.2455	393
0.3047	444
0.3549	479
0.4069	504
0.4594	517
0.5104	523
0.5649	512
0.6017	492
0.6587	468
0.7044	437
0.7480	408
0.7880	348
0.8281	309
0.8680	243
0.9030	194
0.9468	112



AUXILIARY INFORMATION

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

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm<sup>3</sup> glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3949, \rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 802.34, T_b(101.32 \text{ kPa})/\text{K} = 372.39$ .  
2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  
 $n(D, 298.15 \text{ K}) = 1.3811, \rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 883.93, T_b(101.32 \text{ kPa})/\text{K} = 371.92$ .

Errors:  $\delta T/\text{K} = 0.02; \delta x_1 = 0.0005; \delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} < 8$ .

SMOOTHING EQUATION

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

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_d$ , and maximum deviation  $\delta_m$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_d$	$\delta_m$
	$10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$						
298.15	2101.4 (8.4)					6.9	11.9

The standard deviations  $\sigma(a_i)$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E| ; \sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
All direct experimental values equally weighted

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
2. Hernández, P.; Ortega, J. J. Chem. Eng. Data, 1997, 42, 1090.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. J. Chem. Thermodyn., 1985, 17, 1127.

**SELECTED DATA ON MIXTURES**  
International DATA Series\*

2c. EXCESS VOLUME

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

Compiled by Thermodynamics Research Center

Components: 1. 2-Butanol, C<sub>4</sub>H<sub>10</sub>O /78-92-2/  
2. Propyl ethanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> /109-60-4/  
State: Binary system, single-phase liquid; pure components, both liquid  
Variables:  $V^E$ , molar excess volume  
 $x_i$ , mole fraction of component  $i$   
Parameters: T, temperature  
Constants: P, pressure  
Method: Calculation of  $V^E$  from density measurements at constant T and P and variable  $x_i$ ; ref. 1

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

SOURCE OF DATA

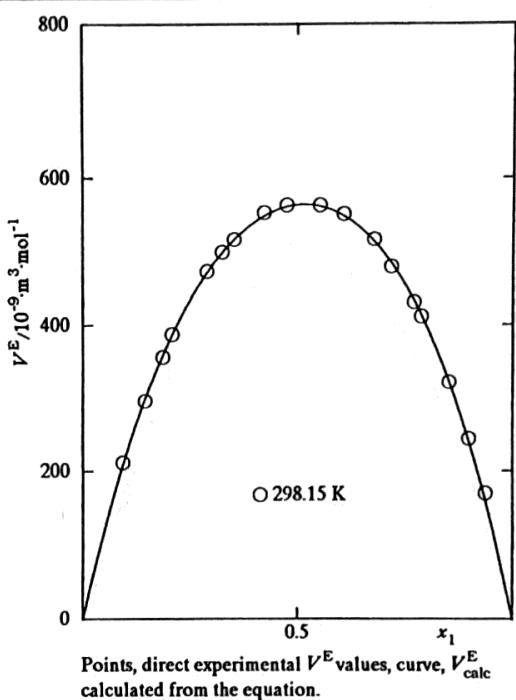
González, C.; Ortega, J.; Hernández, P.; Galván, S. (Laboratorio de Termodinámica y Físicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: P = 101.32 kPa.

T/K = 298.15

$x_1$	$V^E/10^{-9}$ m <sup>3</sup> ·mol <sup>-1</sup>						
0.094	212						
0.146	297						
0.187	357						
0.209	388						
0.290	473						
0.326	500						
0.354	517						
0.423	554						
0.476	564						
0.553	564						
0.608	552						
0.679	517						
0.718	480						
0.771	431						
0.788	412						
0.853	322						
0.899	244						
0.937	170						



AUXILIARY INFORMATION

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

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm<sup>3</sup> glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $n(D, 298.15 \text{ K}) = 1.3949$ ,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 802.58$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 372.27$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $n(D, 298.15 \text{ K}) = 1.3816$ ,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 882.67$ ,  $T_b(101.32 \text{ kPa})/\text{K} = 374.31$ .

Errors:  $\delta T/\text{K} = 0.02$ ;  $\delta x_1 = 0.001$ ;  $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} < 5$ .

SMOOTHING EQUATION

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

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_d$ , and maximum deviation  $\delta_m$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_d$	$\delta_m$
298.15	2262.6 (6.6)	119.9 (11.7)	452 (28)			3.7	9.9

The standard deviations  $\sigma(a_i)$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$ ;  $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
All direct experimental values equally weighted

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
2. González, C.; Ortega, J.; Hernández, P.; Galván, S. J. Chem. Eng. Data, 1999, 44, 772.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. J. Chem. Thermodyn., 1985, 17, 1127.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 2c. EXCESS VOLUME

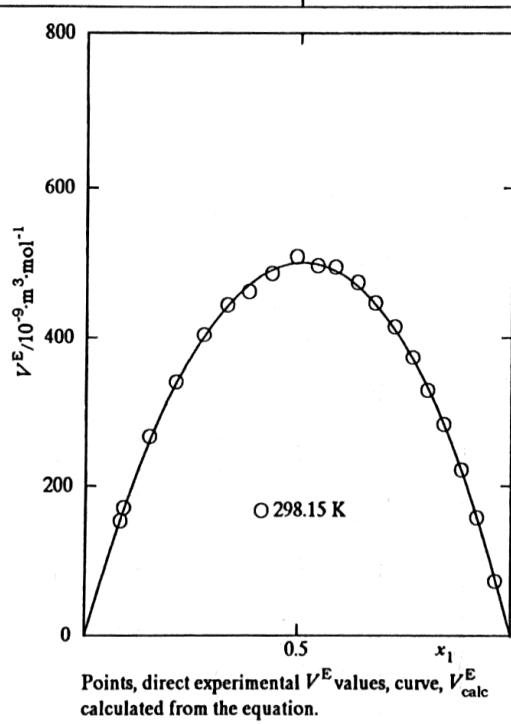
Compiled by Thermodynamics Research Center

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

1047-1503/93/302-1003\$4.00

Components: 1. 2-Butanol, C <sub>4</sub> H <sub>10</sub> O [78-92-2] 2. Ethyl butanone, C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> [105-54-4]	Author(s) of table: Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
State: Binary system, single-phase liquid; pure components, both liquid Variables: $V^E$ , molar excess volume $x_i$ , mole fraction of component $i$ Parameters: $T$ , temperature Constants: $P$ , pressure Method: Calculation of $V^E$ from density measurements at constant $T$ and $P$ and variable $x_i$ ; ref. 1	Edited by: Skrzecz, A.; Maczynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)
<b>SOURCE OF DATA</b>	
Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2	

DIRECT EXPERIMENTAL VALUES					
Notes: $P = 101.32 \text{ kPa}$					
T/K = 298.15					
$x_1$	$V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$	$x_1$	$V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$		
0.0823	155	0.9204	159		
0.0894	172	0.9636	75		
0.1497	266				
0.2112	340				
0.2757	405				
0.3310	445				
0.3814	462				
0.4351	486				
0.4939	508				
0.5433	496				
0.5850	494				
0.6363	474				
0.6791	448				
0.7239	416				
0.7673	373				
0.8038	329				
0.8422	283				
0.8826	222				



AUXILIARY INFORMATION					
Apparatus: The density was determined by an Anton Paar Model DMA-55 vibrating-tube digital densimeter with a precision of $\pm 0.02 \text{ kg} \cdot \text{m}^{-3}$ . The temperature was controlled at $\pm 0.01 \text{ K}$ with a Heto ultrathermostat.					
Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed $2.5 \text{ cm}^3$ glass vials. The apparatus was calibrated with doubly distilled and degassed water and nonane.					
Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3949, \rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 802.34, T_b(101.32 \text{ kPa})/\text{K} = 372.39$ . 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; $n(D, 298.15 \text{ K}) = 1.3898, \rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 873.94, T_b(101.32 \text{ kPa})/\text{K} = 394.18$ .					
Errors: $\delta T/\text{K} = 0.02; \delta x_1 = 0.0005; \delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} < 8$ .					

SMOOTHING EQUATION							
T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_d$	$\delta_m$
	$10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$						
298.15	2004.7 (6.7)	57.2 (13.1)	188 (29)			4.1	10.3

The standard deviations  $\sigma(a_i)$  of the coefficients  $a_i$  are given in parentheses  
 $\delta_m = \max |V_{\text{calc}}^E - V^E|; \sigma_d = [\sum (V_{\text{calc}}^E - V^E)^2 / (N - n)]^{1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_i$   
All direct experimental values equally weighted

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3b, 1994, 22(1).
2. Hernández, P.; Ortega, J. J. Chem. Eng. Data, 1997, 42, 1090.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. J. Chem. Thermodyn., 1985, 17, 1127.