

Components: 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O /71-36-3]2. Butyl methanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> /592-84-7]

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 phasey<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) Gonzales, E.; 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

Gonzales, E.; Ortega, J. (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 <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>	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>	
0.0226	379.28	0.0286	0.7023	383.25	0.5584																
0.0625	379.26	0.0703	0.7368	383.86	0.5940																
0.1288	379.14	0.1289	0.7705	384.58	0.6313																
0.1901	379.16	0.1793	0.8033	385.33	0.6737																
0.2611	379.26	0.2222	0.8492	386.23	0.7278																
0.3066	379.44	0.2582	0.8820	386.90	0.7753																
0.3639	379.63	0.2908	0.9097	387.72	0.8210																
0.4038	379.95	0.3206	0.9478	388.67	0.8888																
0.4396	380.20	0.3471	0.9731	389.44	0.9421																
0.4492	380.29	0.3549	0.9895	389.83	0.9765																
0.4759	380.39	0.3767																			
0.5030	380.63	0.3914																			
0.5290	380.88	0.4118																			
0.5531	381.17	0.4314																			
0.5793	381.49	0.4520																			
0.6063	381.87	0.4740																			
0.6370	382.23	0.5003																			
0.6688	382.70	0.5288																			

## 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 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 vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a digital electronic system (MKS Inst., France).

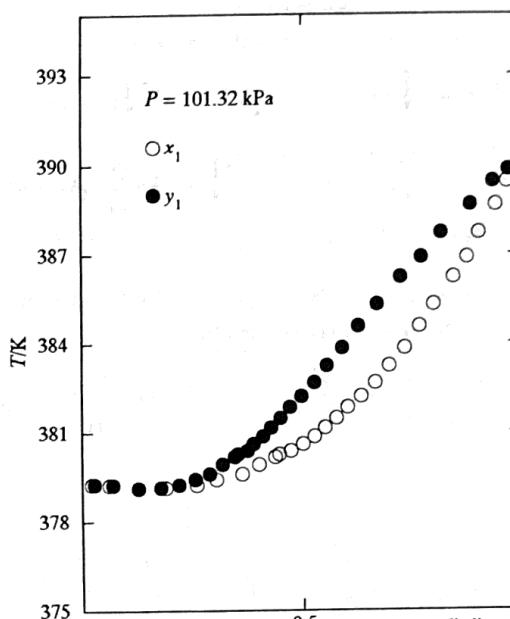
**Procedure:** Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of ±0.01 K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55, vibrating-tube digital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

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification; ρ(298.15 K)/kg·m<sup>-3</sup> = 805.68; n(D, 298.15 K) = 1.3971.

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over

mol. sieve type 3A (Fluka AG), and used without further purification; ρ(298.15 K)/kg·m<sup>-3</sup> = 887.64; n(D, 298.15 K) = 1.3872.

**Errors:** |δT(estd.)|/K = 0.05; |δP(estd.)|/Pa = 50; |δx<sub>1</sub>| = 0.005; |δy<sub>1</sub>| = 0.02.



Points, direct experimental T values.

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

## SELECTED DATA ON MIXTURES

International DATA Series\*

3m. LIQUID-VAPOR EQUILIBRIUM

Published by Thermodynamics Research Center

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

0147-1503/96/0004-248\$4.00

**Components:** 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O [71-36-3]  
2. Butyl methanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> [592-84-7]

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

**Variables:** T, temperature

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

x<sub>i</sub>, mole fraction of component i in liquid 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) of table 3k:** Gonzales, E.; 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)

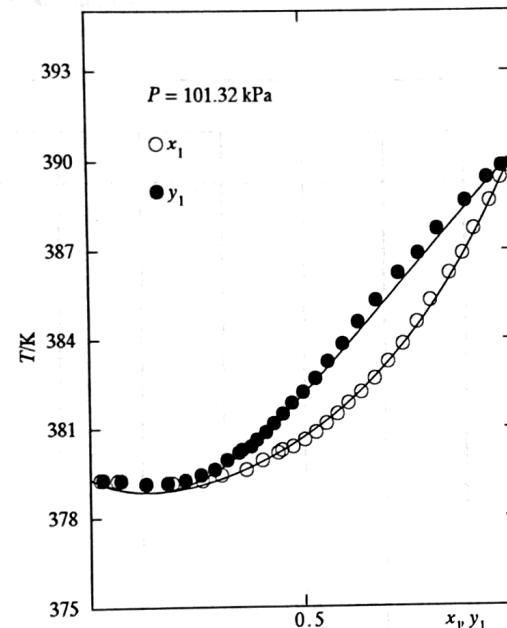
## SOURCE OF DATA

Gonzales, E.; Ortega, J. (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<sub>i</sub>

x <sub>i</sub>	T/K	y <sub>i</sub>				
0.00	379.36	0.0000				
0.05	379.07	0.0563				
0.10	378.93	0.1047				
0.15	378.91	0.1476				
0.20	378.97	0.1869				
0.25	379.12	0.2236				
0.30	379.32	0.2588				
0.40	379.92	0.3278				
0.50	380.75	0.3991				
0.60	381.84	0.4775				
0.70	383.25	0.5683				
0.75	384.09	0.6204				
0.80	385.05	0.6785				
0.85	386.12	0.7437				
0.90	387.33	0.8176				
0.95	388.69	0.9022				
1.00	390.22	1.0000				

Std. dev. σ(T)/K, rel. std. dev. 100σ(δP/P), and abs. max. dev. δ<sub>m</sub>(T)/K at P/kPa = 101.32 are resp.: 0.116, 0.386, 0.203.



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 28 T<sub>exp</sub> data at 101.32 kPa were reduced using the modified Wilson eq., 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 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<sub>ij</sub> (ref. 5) and the molar volumes under saturation pressure V<sub>i</sub><sup>0</sup> (ref. 6).

**Errors:** Std. dev. σ(T) = [Σ(T-T<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,  
Rel. std. dev. 100σ(δP/P) = 100[Σ((P-P<sub>exp</sub>)/P<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,  
N, no. of exp. points, ref. 2,  
n, no. of coefficients in the smoothing equation.

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

P/kPa	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
101.32	7.343 (13.9)	0 (0)	221.03 (18.8)	0 (0)	

The std. deviations σ(a<sub>i</sub>) of the coeffs. 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	15.92700	-3620.84	-70.04	15.02712	-3530.78	-40.15

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Gonzales, E.; Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1996, 24, 247.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5520, 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

Published by Thermodynamics Research Center

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

0147-1503/96/9604-249\$5.00

Components:	1. 1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3] 2. Butyl ethanoate, C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> [123-86-4]
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:	Direct measurement of T, x <sub>i</sub> , and y <sub>i</sub> at constant P; ref. 1

Author(s) Gonzales, E.; 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

Gonzales, E.; Ortega, J. (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 <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>								
0.0430	397.43	0.0804	0.6241	390.07	0.6715								
0.0832	396.59	0.1321	0.6654	389.94	0.6964								
0.1158	395.89	0.1843	0.6966	389.84	0.7219								
0.1551	395.12	0.2335	0.7211	389.76	0.7485								
0.1977	394.42	0.2818	0.7589	389.69	0.7744								
0.2341	393.77	0.3247	0.8019	389.65	0.7990								
0.2731	393.25	0.3623	0.8375	389.72	0.8282								
0.3203	392.60	0.4115	0.8658	389.82	0.8566								
0.3599	392.13	0.4487	0.9108	389.90	0.8933								
0.4036	391.67	0.4874	0.9371	389.96	0.9239								
0.4479	391.29	0.5231	0.9729	390.13	0.9678								
0.4841	390.97	0.5551											
0.5039	390.82	0.5682											
0.5194	390.71	0.5844											
0.5217	390.65	0.5866											
0.5495	390.48	0.6083											
0.5755	390.32	0.6299											
0.6087	390.15	0.6536											

## 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 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 vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a digital electronic system (MKS Inst., France).

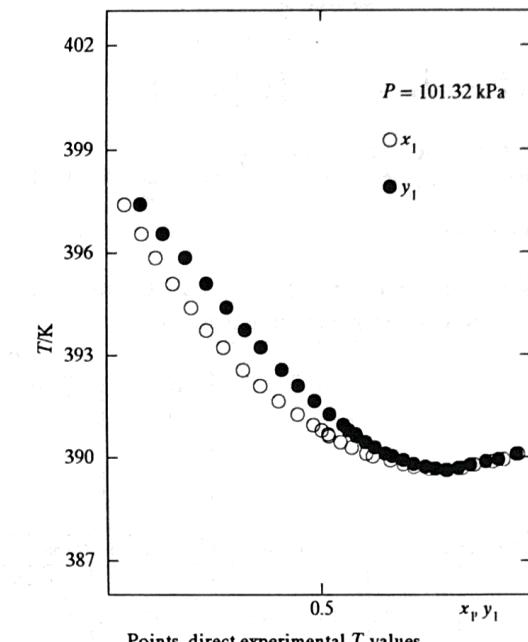
Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of  $\pm 0.01$  K with a digital thermometer, Comark, Model 6900, calibrated against ITS-90. Compositions were determined by densimetric analysis, using an Anton Paar, Model DMA-55 vibrating-tube digital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

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 805.68$ ;  $n(D, 298.15 \text{ K}) = 1.3971$ .  
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 875.89$ ;  $n(D, 298.15 \text{ K}) = 1.3920$ .

Errors:  $|8T(\text{estd.})|/K = 0.05$ ;  $|8P(\text{estd.})|/\text{Pa} = 20$ ;  $|8x_1| = 0.002$ ;  $|8y_1| = 0.01$ .

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.



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## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3m. LIQUID-VAPOR EQUILIBRIUM

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

Published by Thermodynamics Research Center

0147-1503/96/9604-25\$4.00

**Components:** 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O [71-36-3]  
2. Butyl ethanoate, C<sub>6</sub>H<sub>12</sub>O<sub>2</sub> [123-86-4]

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

**Variables:** T, temperature

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

x<sub>i</sub>, mole fraction of component i in liquid phase

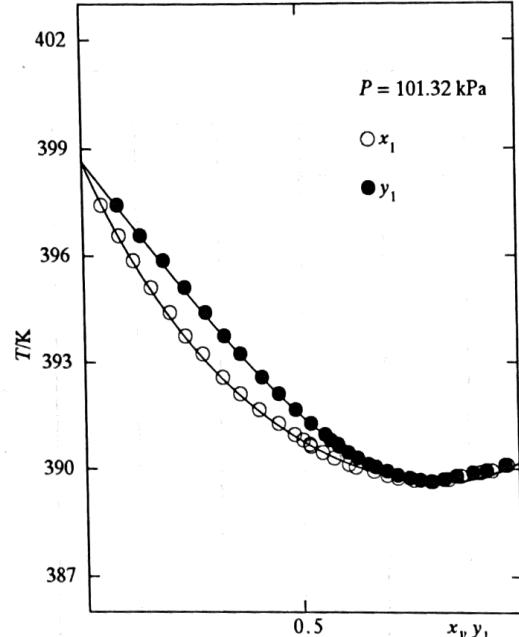
**Parameters:** P, pressure

**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

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

x <sub>i</sub>	T/K	y <sub>i</sub>				
0.00	398.69	0.0000				
0.05	397.36	0.0839				
0.10	396.21	0.1585				
0.15	395.19	0.2256				
0.20	394.30	0.2864				
0.25	393.52	0.3421				
0.30	392.83	0.3936				
0.40	391.70	0.4866				
0.50	390.85	0.5701				
0.60	390.24	0.6480				
0.70	389.85	0.7243				
0.75	389.73	0.7631				
0.80	389.68	0.8034				
0.85	389.68	0.8458				
0.90	389.76	0.8917				
0.95	389.94	0.9424				
1.00	390.22	1.0000				

Std. dev. σ(T)/K, rel. std. dev. 100σ(δP/P), and abs. max. dev. δ<sub>m</sub>(T)/K  
at P/kPa = 101.32 are resp.: 0.052, 0.175, 0.115.



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 29 T<sub>exp</sub> data at 101.32 kPa were reduced using the modified Wilson eq., 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 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<sub>ij</sub> (ref. 5) and the molar volumes under saturation pressure V<sub>i</sub><sup>0</sup> (ref. 6).

**Errors:** Std. dev. σ(T) = [Σ(T - T<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,  
Rel. std. dev. 100σ(δP/P) = 100[Σ((P - P<sub>exp</sub>)/P<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,  
N, no. of exp. points, ref. 2,  
n, no. of coefficients in the smoothing equation.

**Author(s)** Gonzales, E.; 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

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

P/kPa	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
101.32	249.69 (10.9)	0 (0)	-60.523 (7.3)	0 (0)	

The std. deviations σ(a<sub>i</sub>) of the coeffs. 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	15.92700	-3620.84	-70.04	14.97940	-3676.54	-43.85

## REFERENCES

- Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
- Gonzales, E.; Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1996, 24, 249.
- Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
- TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5550, 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

Published by Thermodynamics Research Center

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

0147-1503/96/9604-251\$4.00

Components:	1. 1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3] 2. Butyl propanoate, C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> [590-01-2]	Author(s)	Gonzales, E.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor	Edited by:	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>i</i> in liquid phase		
	y <sub>i</sub> , mole fraction of component <i>i</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  
Gonzales, E.; Ortega, J. (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 <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>
0.0382	415.49	0.1110	0.6857	394.07	0.8090
0.0885	412.38	0.2335	0.6861	394.06	0.8098
0.1411	409.72	0.3341	0.7078	393.75	0.8202
0.1938	407.31	0.4136	0.7270	393.40	0.8318
0.2573	404.76	0.4904	0.7691	392.85	0.8556
0.3201	402.58	0.5549	0.8120	392.31	0.8804
0.3769	400.81	0.6044	0.8554	391.72	0.9055
0.4241	399.34	0.6446	0.8973	391.30	0.9310
0.4697	398.18	0.6785	0.9380	390.85	0.9570
0.5107	397.18	0.7077	0.9643	390.78	0.9768
0.5476	396.43	0.7306			
0.5479	396.38	0.7309			
0.5831	395.79	0.7524			
0.6008	395.54	0.7604			
0.6144	395.26	0.7711			
0.6434	394.84	0.7851			
0.6440	394.79	0.7854			
0.6627	394.44	0.7968			

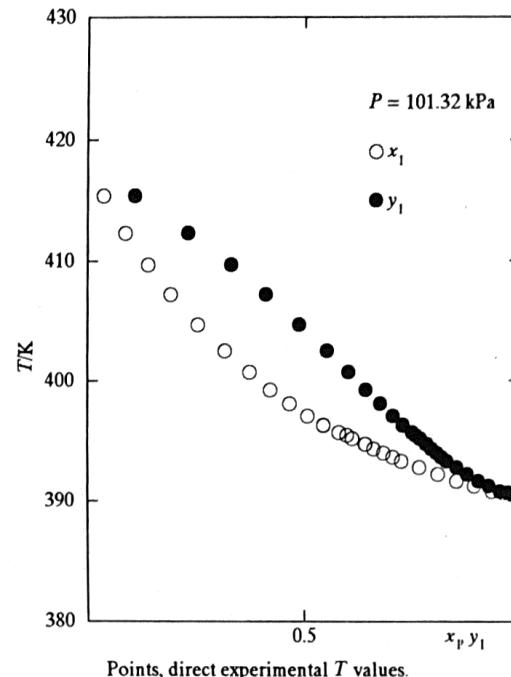
## AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 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 vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a digital electronic system (MKS Inst., France).

Procedure: Operation described in ref. 3. The equilibrium temperatures were measured with an accuracy of  $\pm 0.01$  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), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 805.68$ ;  $n(D, 298.15 \text{ K}) = 1.3971$ .  
2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 871.12$ ;  $n(D, 298.15 \text{ K}) = 1.3989$ .

Errors:  $|\delta T(\text{estd.})|/K = 0.05$ ;  $|\delta P(\text{estd.})|/\text{Pa} = 20$ ;  $|\delta x_1| = 0.002$ ;  $|\delta y_1| = 0.01$ .



Points, direct experimental T values.

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
3. Ortega, J.; Pena, J. A.; de Alfonso, C. J. Chem. Eng. Data 1986, 31, 339.

Components: 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O /71-36-3/2. Butyl propanoate, C<sub>7</sub>H<sub>14</sub>O<sub>2</sub> /590-01-2/

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

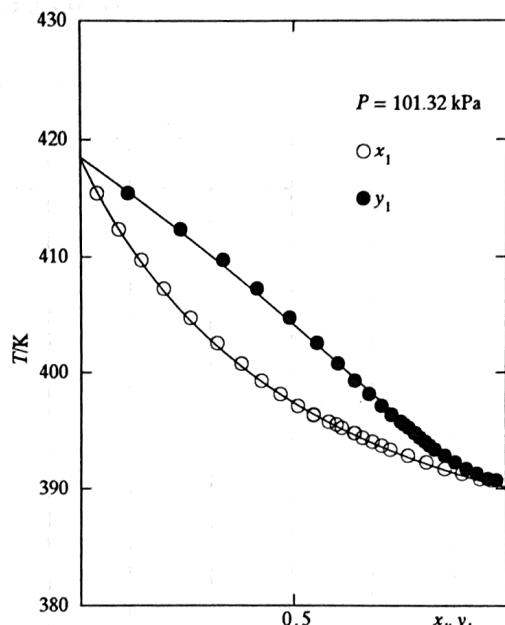
Variables: T, temperature

y<sub>i</sub>, mole fraction of component i in vapor phasex<sub>i</sub>, mole fraction of component i in liquid 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. 1Notes: The table reports smoothed values of T and calcd. values of y<sub>i</sub>

x <sub>i</sub>	T/K	y <sub>i</sub>				
0.00	418.60	0.0000				
0.05	414.98	0.1365				
0.10	411.90	0.2467				
0.15	409.25	0.3378				
0.20	406.94	0.4145				
0.25	404.90	0.4803				
0.30	403.10	0.5373				
0.40	400.04	0.6322				
0.50	397.56	0.7087				
0.60	395.53	0.7732				
0.70	393.84	0.8302				
0.75	393.10	0.871				
0.80	392.42	0.8836				
0.85	391.79	0.9103				
0.90	391.22	0.9379				
0.95	390.70	0.9673				
1.00	390.22	1.0000				

Std. dev. σ(T)/K, rel. std. dev. 100σ(δP/P), and abs. max. dev. δ<sub>m</sub>(T)/K  
at P/kPa = 101.32 are resp.: 0.107, 0.337, 0.218.Points, direct experimental T values, curves, T(x<sub>1</sub>) and T(y<sub>1</sub>), calculated from the equations.

Author(s) Gonzales, E.; 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

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

## EQUATIONS

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

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

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

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

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

## COEFFICIENTS IN THE EQUATIONS

P/kPa	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
101.32	328.47 (18.8)	0 (0)	-121.5 (10.9)	0 (0)	

The std. deviations σ(a<sub>i</sub>) of the coeffs. 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	15.92700	-3620.84	-70.04	13.46639	-2837.50	-97.91

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).
2. Gonzales, E.; Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1996, 24, 251.
3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.
4. TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1976, k-5000, 1969, k-5580, 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.

## AUXILIARY INFORMATION

Measurements: The T<sub>exp</sub> data at 101.32 kPa are reported in ref. 2.Computations: The 28 T<sub>exp</sub> data at 101.32 kPa were reduced using the modified Wilson eq., 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 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<sub>ij</sub> (ref. 5) and the molar volumes under saturation pressure V<sub>i</sub><sup>0</sup> (ref. 6).Errors: Std. dev. σ(T) = [Σ(T-T<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,Rel. std. dev. 100σ(δP/P) = 100[Σ((P-P<sub>exp</sub>)/P<sub>exp</sub>)<sup>2</sup>/(N-n)]<sup>1/2</sup>,

N, no. of exp. points, ref. 2,

n, no. of coefficients in the smoothing equation.

## SELECTED DATA ON MIXTURES

International DATA Series\*

## 3k. LIQUID-VAPOR EQUILIBRIUM

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

Published by Thermodynamics Research Center

0147-1503/96/69604-25\$34.00

Components: 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O /71-36-3/2. Butyl butanoate, C<sub>8</sub>H<sub>16</sub>O<sub>2</sub> /109-21-7/

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 phasey<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) Gonzales, E.; 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

Gonzales, E.; Ortega, J. (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 <sub>1</sub>	T/K	y <sub>1</sub>	x <sub>1</sub>	T/K	y <sub>1</sub>														
0.0340	434.81	0.1453	0.6717	396.86	0.8849														
0.0625	431.30	0.2436	0.7109	395.93	0.8990														
0.1042	426.80	0.3604	0.7574	394.76	0.9175														
0.1424	423.23	0.4455	0.7992	394.05	0.9297														
0.1879	419.38	0.5259	0.8358	393.29	0.9423														
0.2313	416.15	0.5826	0.8677	392.66	0.9528														
0.2739	413.25	0.6318	0.8998	392.04	0.9639														
0.3131	410.67	0.6743	0.9313	391.49	0.9749														
0.3535	408.58	0.7087	0.9656	390.87	0.9870														
0.3893	406.88	0.7367	0.9734	390.79	0.9896														
0.4381	404.81	0.7686																	
0.4767	403.08	0.7923																	
0.5172	401.62	0.8135																	
0.5554	400.29	0.8322																	
0.5574	400.21	0.8332																	
0.5840	399.36	0.8456																	
0.6096	398.45	0.8586																	
0.6204	398.29	0.8616																	

## AUXILIARY INFORMATION

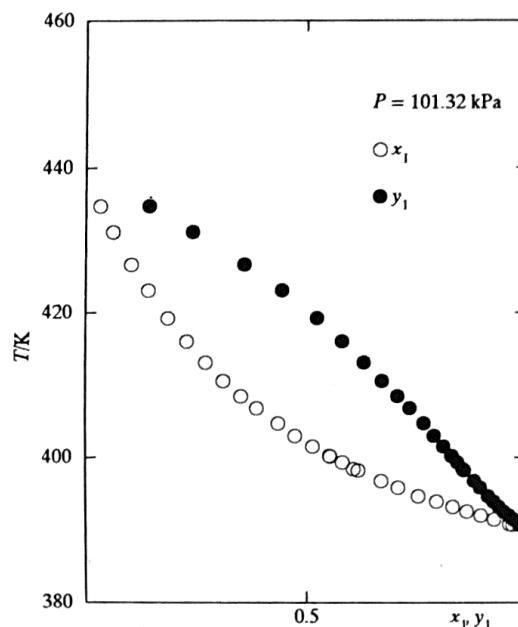
Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of approx. 50 cm<sup>3</sup>, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Normschliff Gerätebau Wertheim) and measured with a digital electronic system (MKS Inst., France).

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## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 3k, 1994, 22(4).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
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## SELECTED DATA ON MIXTURES

International DATA Series\*

3m. LIQUID-VAPOR EQUILIBRIUM

Published by Thermodynamics Research Center

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

0147-1503/96/9604-25\$4.00

<b>Components:</b> 1. 1-Butanol, C <sub>4</sub> H <sub>10</sub> O /71-36-3/ 2. Butyl butanoate, C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> /109-21-7/			<b>Author(s)</b> Gonzales, E.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)																																																																				
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<b>Variables:</b> T, temperature $y_i$ , mole fraction of component i in vapor phase $x_i$ , mole fraction of component i in liquid phase			<b>SOURCE OF DATA</b>																																																																				
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<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; padding: 2px;">x<sub>i</sub></th> <th style="text-align: left; padding: 2px;">T/K</th> <th style="text-align: left; padding: 2px;">y<sub>i</sub></th> </tr> </thead> <tbody> <tr><td style="text-align: left; padding: 2px;">0.00</td><td style="text-align: left; padding: 2px;">439.48</td><td style="text-align: left; padding: 2px;">0.0000</td></tr> <tr><td style="text-align: left; padding: 2px;">0.05</td><td style="text-align: left; padding: 2px;">432.67</td><td style="text-align: left; padding: 2px;">0.2050</td></tr> <tr><td style="text-align: left; padding: 2px;">0.10</td><td style="text-align: left; padding: 2px;">427.06</td><td style="text-align: left; padding: 2px;">0.3528</td></tr> <tr><td style="text-align: left; padding: 2px;">0.15</td><td style="text-align: left; padding: 2px;">422.33</td><td style="text-align: left; padding: 2px;">0.4636</td></tr> <tr><td style="text-align: left; padding: 2px;">0.20</td><td style="text-align: left; padding: 2px;">418.27</td><td style="text-align: left; padding: 2px;">0.5495</td></tr> <tr><td style="text-align: left; padding: 2px;">0.25</td><td style="text-align: left; padding: 2px;">414.75</td><td style="text-align: left; padding: 2px;">0.6178</td></tr> <tr><td style="text-align: left; padding: 2px;">0.30</td><td style="text-align: left; padding: 2px;">411.66</td><td style="text-align: left; padding: 2px;">0.6735</td></tr> <tr><td style="text-align: left; padding: 2px;">0.40</td><td style="text-align: left; padding: 2px;">406.48</td><td style="text-align: left; padding: 2px;">0.7585</td></tr> <tr><td style="text-align: left; padding: 2px;">0.50</td><td style="text-align: left; padding: 2px;">402.31</td><td style="text-align: left; padding: 2px;">0.8205</td></tr> <tr><td style="text-align: left; padding: 2px;">0.60</td><td style="text-align: left; padding: 2px;">398.91</td><td style="text-align: left; padding: 2px;">0.8677</td></tr> <tr><td style="text-align: left; padding: 2px;">0.70</td><td style="text-align: left; padding: 2px;">396.13</td><td style="text-align: left; padding: 2px;">0.9053</td></tr> <tr><td style="text-align: left; padding: 2px;">0.75</td><td style="text-align: left; padding: 2px;">394.93</td><td style="text-align: left; padding: 2px;">0.9216</td></tr> <tr><td style="text-align: left; padding: 2px;">0.80</td><td style="text-align: left; padding: 2px;">393.85</td><td style="text-align: left; padding: 2px;">0.9368</td></tr> <tr><td style="text-align: left; padding: 2px;">0.85</td><td style="text-align: left; padding: 2px;">392.85</td><td style="text-align: left; padding: 2px;">0.9514</td></tr> <tr><td style="text-align: left; padding: 2px;">0.90</td><td style="text-align: left; padding: 2px;">391.93</td><td style="text-align: left; padding: 2px;">0.9659</td></tr> <tr><td style="text-align: left; padding: 2px;">0.95</td><td style="text-align: left; padding: 2px;">391.07</td><td style="text-align: left; padding: 2px;">0.9815</td></tr> <tr><td style="text-align: left; padding: 2px;">1.00</td><td style="text-align: left; padding: 2px;">390.22</td><td style="text-align: left; padding: 2px;">1.0000</td></tr> </tbody> </table>			x <sub>i</sub>	T/K	y <sub>i</sub>	0.00	439.48	0.0000	0.05	432.67	0.2050	0.10	427.06	0.3528	0.15	422.33	0.4636	0.20	418.27	0.5495	0.25	414.75	0.6178	0.30	411.66	0.6735	0.40	406.48	0.7585	0.50	402.31	0.8205	0.60	398.91	0.8677	0.70	396.13	0.9053	0.75	394.93	0.9216	0.80	393.85	0.9368	0.85	392.85	0.9514	0.90	391.93	0.9659	0.95	391.07	0.9815	1.00	390.22	1.0000	<b>COEFFICIENTS IN THE EQUATIONS</b> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; padding: 2px;">P/kPa</th> <th style="text-align: left; padding: 2px;"><math>a_1</math></th> <th style="text-align: left; padding: 2px;"><math>a_2</math></th> <th style="text-align: left; padding: 2px;"><math>a_3</math></th> <th style="text-align: left; padding: 2px;"><math>a_4</math></th> <th style="text-align: left; padding: 2px;"><math>a_5</math></th> </tr> </thead> <tbody> <tr><td style="text-align: left; padding: 2px;">101.32</td><td style="text-align: left; padding: 2px;">556.95 (19.1)</td><td style="text-align: left; padding: 2px;">0 (0)</td><td style="text-align: left; padding: 2px;">-241.2 (6.7)</td><td style="text-align: left; padding: 2px;">0 (0)</td><td></td></tr> </tbody> </table>			P/kPa	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	101.32	556.95 (19.1)	0 (0)	-241.2 (6.7)	0 (0)	
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P/kPa	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$																																																																		
101.32	556.95 (19.1)	0 (0)	-241.2 (6.7)	0 (0)																																																																			
Std. dev. $\sigma(T)/K$ , rel. std. dev. 100 $\sigma(\delta P/P)$ , and abs. max. dev. $\delta_m(T)/K$ at $P/kPa = 101.32$ are resp.: 0.125, 0.395, 0.232.			The std. deviations $\sigma(a_i)$ of the coeffs. $a_i$ are given in parentheses. <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; padding: 2px;">P/kPa</th> <th style="text-align: left; padding: 2px;"><math>A_1</math></th> <th style="text-align: left; padding: 2px;"><math>B_1</math></th> <th style="text-align: left; padding: 2px;"><math>C_1</math></th> <th style="text-align: left; padding: 2px;"><math>A_2</math></th> <th style="text-align: left; padding: 2px;"><math>B_2</math></th> <th style="text-align: left; padding: 2px;"><math>C_2</math></th> </tr> </thead> <tbody> <tr><td style="text-align: left; padding: 2px;">101.32</td><td style="text-align: left; padding: 2px;">15.92700</td><td style="text-align: left; padding: 2px;">-3620.84</td><td style="text-align: left; padding: 2px;">-70.04</td><td style="text-align: left; padding: 2px;">20.01861</td><td style="text-align: left; padding: 2px;">-8687.73</td><td style="text-align: left; padding: 2px;">124.65</td></tr> </tbody> </table>			P/kPa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$	101.32	15.92700	-3620.84	-70.04	20.01861	-8687.73	124.65																																																				
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<b>AUXILIARY INFORMATION</b> <b>Measurements:</b> The $T_{\exp}$ data at 101.32 kPa are reported in ref. 2.			<b>REFERENCES</b> <ol style="list-style-type: none"> <li>1. Int. DATA Ser., Ser. A, Guideline 3m, 1995, 23(2).</li> <li>2. Gonzales, E.; Ortega, J. Int. DATA Ser., Sel. Data Mixtures, Ser. A 1996, 24, 253.</li> <li>3. Wilson, G. M. J. Am. Chem. Soc. 1964, 86, 127.</li> <li>4. TRC Thermodynamic Tables - Hydrocarbons &amp; Non-Hydrocarbons, 1976, k-5000, 1978, k-5520, Thermodynamics Research Center, The Texas A&amp;M University System, College Station, TX, USA.</li> <li>5. Tsionopoulos, C. AIChE J. 1974, 20, 263; 1975, 21, 827.</li> <li>6. Yen, L. C.; Woods, S. S. AIChE J. 1966, 12, 95.</li> </ol>																																																																				
<b>Computations:</b> 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 $\mu_i^E$ .																																																																							
<b>Corrections:</b> Vapor pressure equation parameters were taken from refs. 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).																																																																							
<b>Errors:</b> Std. dev. $\sigma(T) = [\sum(T - T_{\exp})^2/(N-n)]^{1/2}$ , Rel. std. dev. 100 $\sigma(\delta P/P) = 100[\sum((P - P_{\exp})/P_{\exp})^2/(N-n)]^{1/2}$ , $N$ , no. of exp. points, ref. 2, $n$ , no. of coefficients in the smoothing equation.																																																																							

Received: September 15, 1996

Published: October 31, 1996

Components: 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O [71-36-3]2. Butyl methanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> [592-84-7]

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

Variables: V<sup>E</sup>, molar excess volumex<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

Author(s) Gonzales, E.; 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

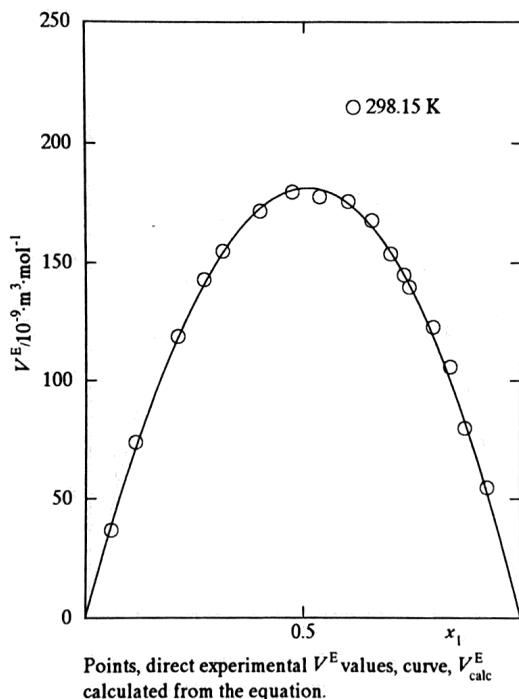
Gonzales, E.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

Notes: P, atm.

T/K = 298.15

x <sub>1</sub>	V <sup>E</sup> /10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>					
0.0584	37					
0.1141	74					
0.2107	119					
0.2709	143					
0.3144	155					
0.3998	172					
0.4743	180					
0.5362	178					
0.6030	176					
0.6568	168					
0.7006	154					
0.7304	145					
0.7424	140					
0.7991	123					
0.8380	106					
0.8718	80					
0.9226	55					



## AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter type DMA 55 equipped with a cell model 602, (Anton-Paar, Graz, Austria). Temperature was controlled to within 0.01 K with a Heto Thermostat and was measured by means of a calibrated Pt thermometer.

Procedure: Density, ρ, was calcd. from period of vibration, τ: ρ = a + bτ<sup>2</sup>. Consts. a and b were detd. by calibrating the app. (ref. 3) with doubly distd. and degassed H<sub>2</sub>O, ρ(298.15 K)/kg·m<sup>-3</sup> = 997.043 (ref. 4), and nonane (Fluka AG), "purum" grade material of stated purity > 99 mole %, ρ(298.15 K)/kg·m<sup>-3</sup> = 713.855 (ref. 5). Mixtures were prep'd. by mass. V<sup>E</sup> was calcd. from V<sup>E</sup> = V - (x<sub>1</sub>V<sub>1</sub><sup>0</sup> + x<sub>2</sub>V<sub>2</sub><sup>0</sup>), where V = (x<sub>1</sub>M<sub>1</sub> + x<sub>2</sub>M<sub>2</sub>)/ρ is the molar vol. of the mixt. and V<sub>i</sub><sup>0</sup> = V(x<sub>i</sub> = 1) and M<sub>i</sub> are resp., the molar vol. and molar mass of component i.Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification; ρ(298.15 K)/kg·m<sup>-3</sup> = 805.68; n(D, 298.15 K) = 1.3971.

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity &gt; 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification.

Errors: δT(reproducibility)/K = 0.01; δT(ITS-90)/K = 0.01; δx<sub>1</sub> = 0.0001; δV<sup>E</sup>/10<sup>-9</sup> m<sup>3</sup>·mol<sup>-1</sup> = 2.

## SMOOTHING EQUATION

$$V_{\text{calc}}^E = x_1 x_2 a_1 / \left[ 1 + \sum_{i=2}^n a_i (x_1 - x_2)^{i-1} \right]$$

Coeffs. a<sub>i</sub> in the smoothing eq., std. deviation σ<sub>d</sub>, and max. deviation δ<sub>m</sub> detd. by least-squares anal.

T/K	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	σ <sub>d</sub>	δ <sub>m</sub>
	10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>						
298.15	727.49 (3.17)	-0.039 (0.011)				2.4	4.6

The std. deviations σ<sub>a<sub>i</sub></sub> of the coeffs. a<sub>i</sub> are given in parentheses  
δ<sub>m</sub> = max |V<sub>calc</sub><sup>E</sup> - V<sup>E</sup>| ; σ<sub>d</sub> = [Σ(V<sub>calc</sub><sup>E</sup> - V<sup>E</sup>)<sup>2</sup>/(N - n)]<sup>1/2</sup>N, no. of direct exptl. values; n, no. of coeffs. a<sub>i</sub>

All direct exptl. values equally weighted

## REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 2c, 1994, 22(1).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jimenez, E. J. J. Chem. Thermodyn. 1985, 17, 1127.
4. Riddick, J. A.; Bunger, W. B.; Sakano, T. K. Organic Solvents. Techniques of Chemistry, Vol. II. 4th ed., Wiley-Interscience, New York, 1986.
5. Anton Paar Information Bull. No. 6, March 1982.

**SELECTED DATA ON MIXTURES**  
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2c. EXCESS VOLUME

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0147-1503/96/9604-256\$4.00

Components: 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O /71-36-3/  
2. Butyl ethanoate, C<sub>6</sub>H<sub>12</sub>O<sub>2</sub> /123-86-4/

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

Variables: V<sup>E</sup>, molar excess volume  
 $x_i$ , 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  $x_i$ ; ref. 1

Author(s) Gonzales, E.; 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

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

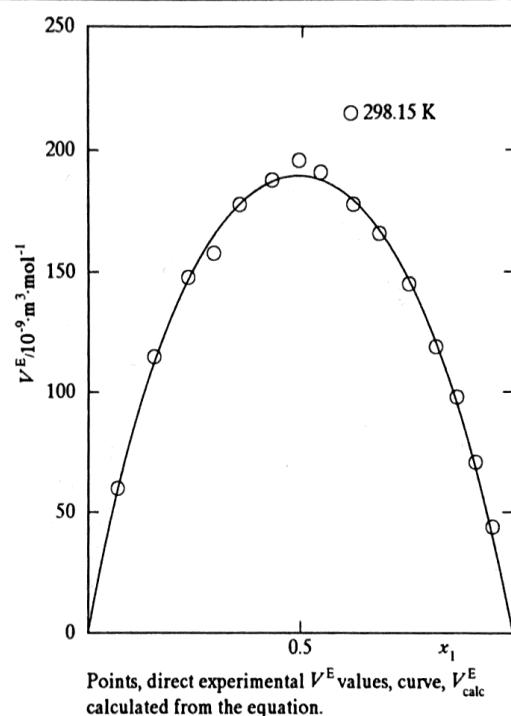
DIRECT EXPERIMENTAL VALUES

Notes: P, atm.

T/K = 298.15

$x_1$        $V^E/10^{-9}$   
m<sup>3</sup>·mol<sup>-1</sup>

0.0691	60
0.1559	115
0.2359	148
0.2959	158
0.3555	178
0.4313	188
0.4938	196
0.5448	191
0.6216	178
0.6838	166
0.7534	145
0.8185	119
0.8670	98
0.9121	71
0.9525	44



AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter type DMA 55 equipped with a cell model 602, (Anton-Paar, Graz, Austria). Temperature was controlled to within 0.01 K with a Heto Thermostat and was measured by means of a calibrated Pt thermometer.

Procedure: Density,  $\rho$ , was calcd. from period of vibration,  $\tau$ :  $\rho = a + b\tau^2$ . Consts.  $a$  and  $b$  were detd. by calibrating the app. (ref. 3) with doubly distd. and degassed H<sub>2</sub>O,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 997.043$  (ref. 4), and nonane (Fluka AG), "purum" grade material of stated purity > 99 mole %,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 713.855$  (ref. 5). Mixtures were prep'd. by mass.  $V^E$  was calcd. from  $V^E = V - (x_1 V_1^0 + x_2 V_2^0)$ , where  $V = (x_1 M_1 + x_2 M_2)/\rho$  is the molar vol. of the mixt. and  $V_i^0 = V(x_i = 1)$  and  $M_i$  are resp., the molar vol. and molar mass of component *i*.

Materials: 1. Fluka AG (Buchs St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 805.68$ ;  $n(D, 298.15 \text{ K}) = 1.3971$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification.

Errors:  $\delta T(\text{reproducibility})/K = 0.01$ ;  $\delta T(\text{ITS-90})/K = 0.01$ ;  $\delta x_i = 0.0001$ ;  $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} = 2$ .

SMOOTHING EQUATION

$$V_{\text{calc}}^E = x_1 x_2 a_1 / [1 + \sum_{i=2}^n a_i (x_1 - x_2)^{i-1}]$$

Coeffs.  $a_i$  in the smoothing eq., std. deviation  $\sigma_d$ , and max. deviation  $\delta_m$  detd. by least-squares anal.

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	759.9 (6.1)	0.022 (0.015)	-0.205 (0.033)			3.4	7.5

The std. deviations  $\sigma_a$  of the coeffs.  $a_i$  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, no. of direct exptl. values; n, no. of coeffs.  $a_i$

All direct exptl. values equally weighted

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 2c, 1994, 22(1).
2. Gonzales, E.; Ortega, J. J. Chem. Eng. Data, 1996, 41, 53.
3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jimenez, E. J. J. Chem. Thermodyn. 1985, 17, 1127.
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5. Anton Paar Information Bull. No. 6, March 1982.

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2c. EXCESS VOLUME

**Components:** 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O [71-36-3]  
2. Butyl propanoate, C<sub>7</sub>H<sub>14</sub>O<sub>2</sub> [590-01-2]  
**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

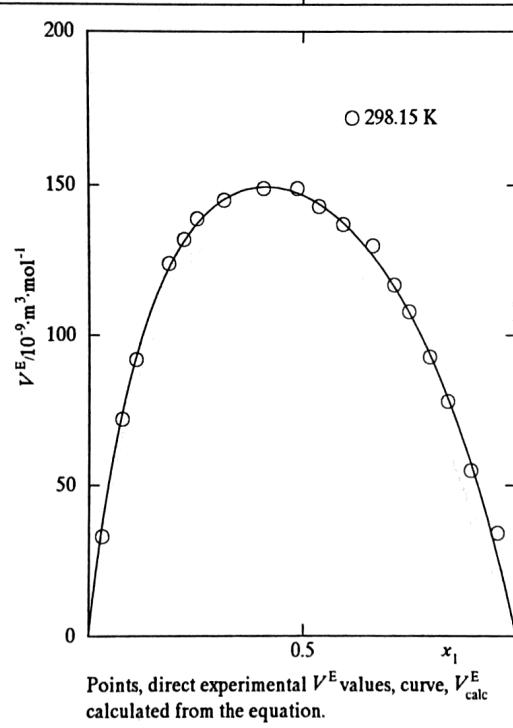
**Author(s)** Gonzales, E.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain)

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

SOURCE OF DATA

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

DIRECT EXPERIMENTAL VALUES	
Notes: P, atm.	
T/K = 298.15	
x <sub>1</sub>	V <sup>E</sup> /10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>
0.0314	33
0.0767	72
0.1091	92
0.1864	124
0.2223	132
0.2527	139
0.3149	145
0.4076	149
0.4866	149
0.5373	143
0.5937	137
0.6626	130
0.7143	117
0.7496	108
0.7982	93
0.8418	78
0.8951	55
0.9576	34



SMOOTHING EQUATION

$$V_{\text{calc}}^E = x_1 x_2 a_1 / \left[ 1 + \sum_{i=2}^n a_i (x_1 - x_2)^{i-1} \right]$$

Coeffs. a<sub>i</sub> in the smoothing eq., std. deviation σ<sub>d</sub>, and max deviation δ<sub>m</sub> detd. by least-squares anal.

T/K	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	σ <sub>d</sub>	δ <sub>m</sub>
	10 <sup>-9</sup> m <sup>3</sup> ·mol <sup>-1</sup>						
298.15	588.1 (4.6)	0.215 (0.013)	-0.350 (0.027)			2.6	7.6

The std. deviations σ<sub>a<sub>i</sub></sub> of the coeffs. a<sub>i</sub> 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, no. of direct exptl. values; n, no. of coeffs. a<sub>i</sub>

All direct exptl. values equally weighted

AUXILIARY INFORMATION	
<b>Apparatus:</b>	Vibrating tube densimeter type DMA 55 equipped with a cell model 602, (Anton-Paar, Graz, Austria). Temperature was controlled to within 0.01 K with a Heto Thermostat and was measured by means of a calibrated Pt thermometer.
<b>Procedure:</b>	Density, ρ, was calcd. from period of vibration, τ: $\rho = a + b\tau^2$ . Consts. a and b were detd. by calibrating the app. (ref. 3) with doubly distd. and degassed H <sub>2</sub> O, $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 997.043$ (ref. 4), and nonane (Fluka AG), "purum" grade material of stated purity > 99 mole %, $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 713.855$ (ref. 5). Mixtures were prep'd. by mass. V <sup>E</sup> was calcd. from $V^E = V - (x_1 V_1^0 + x_2 V_2^0)$ , where $V = (x_1 M_1 + x_2 M_2)/\rho$ is the molar vol. of the mixt. and $V_i^0 = V(x_i = 1)$ and $M_i$ are resp., the molar vol. and molar mass of component i.
<b>Materials:</b>	1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification; $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 805.68$ ; n(D, 298.15 K) = 1.3971. 2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification.
<b>Errors:</b>	$\delta T(\text{reproducibility})/K = 0.01$ ; $\delta T(\text{ITS-90})/K = 0.01$ ; $\delta x_1 = 0.0001$ ; $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} = 2$ .

REFERENCES

1. Int. DATA Ser., Ser. A, Guideline 2c, 1994, 22(1).
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3. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jimenez, E. J. J. Chem. Thermodyn. 1985, 17, 1127.
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**Components:** 1. 1-Butanol, C<sub>4</sub>H<sub>10</sub>O [71-36-3]  
 2. Butyl butanoate, C<sub>8</sub>H<sub>16</sub>O<sub>2</sub> [109-21-7]

**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:** Gonzales, E.; 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

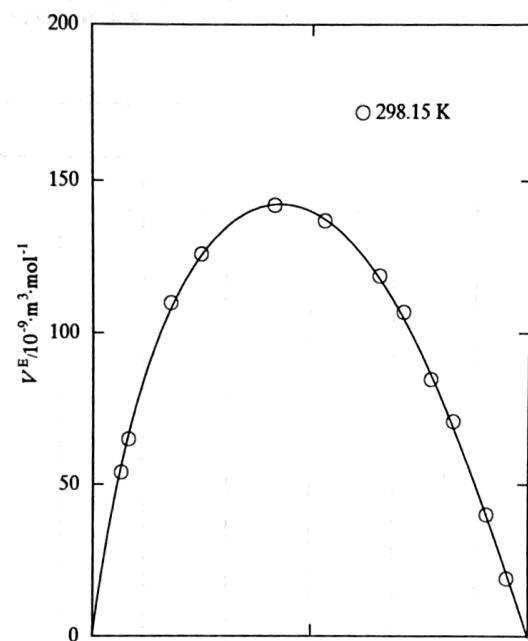
Gonzales, E.; Ortega, J. (Laboratorio de Termodinamica y Fisicoquimica, 35071 -University of Las Palmas de G. C., Canary Islands, Spain); ref. 2

## DIRECT EXPERIMENTAL VALUES

Notes:  $P$ , atm.

T/K = 298.15

$x_1$	$V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1}$					
0.0651	54					
0.0815	65					
0.1778	110					
0.2472	126					
0.4158	142					
0.5286	137					
0.6559	119					
0.7108	107					
0.7753	85					
0.8277	71					
0.9053	40					
0.9514	19					



Points, direct experimental  $V^E$  values, curve,  $V^E_{\text{calc}}$  calculated from the equation.

## AUXILIARY INFORMATION

**Apparatus:** Vibrating tube densimeter type DMA 55 equipped with a cell model 602, (Anton-Paar, Graz, Austria). Temperature was controlled to within 0.01 K with a Heto Thermostat and was measured by means of a calibrated Pt thermometer.

**Procedure:** Density,  $\rho$ , was calcd. from period of vibration,  $\tau$ :  $\rho = a + b\tau^2$ . Consts.  $a$  and  $b$  were detd. by calibrating the app. (ref. 3) with doubly distd. and degassed H<sub>2</sub>O,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 997.043$  (ref. 4), and nonane (Fluka AG), "purum" grade material of stated purity > 99 mole %,  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 713.855$  (ref. 5). Mixtures were prep'd. by mass.  $V^E$  was calcd. from  $V^E = V - (x_1 V_1^0 + x_2 V_2^0)$ , where  $V = (x_1 M_1 + x_2 M_2)/\rho$  is the molar vol. of the mixt. and  $V_i^0 = V(x_i = 1)$  and  $M_i$  are resp., the molar vol. and molar mass of component  $i$ .

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification;  $\rho(298.15 \text{ K})/\text{kg} \cdot \text{m}^{-3} = 805.68$ ;  $n(D, 298.15 \text{ K}) = 1.3971$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), "puriss." grade material of stated GLC purity > 99.5 mole %, degassed with ultrasound, dried over mol. sieve type 3A (Fluka AG), and used without further purification.

**Errors:**  $\delta T(\text{reproducibility})/K = 0.01$ ;  $\delta T(\text{ITS-90})/K = 0.01$ ;  $\delta x_i = 0.0001$ ;  $\delta V^E/10^{-9} \text{ m}^3 \cdot \text{mol}^{-1} = 2$ .

## SMOOTHING EQUATION

$$V^E_{\text{calc}} = x_1 x_2 a_1 / [1 + \sum_{i=2}^n a_i (x_1 - x_2)^{i-1}]$$

Coeffs.  $a_i$  in the smoothing eq., std. deviation  $\sigma_d$ , and max. deviation  $\delta_m$  detd. by least-squares anal.

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	561.2 (4.1)	0.242 (0.024)	-0.109 (0.027)	0.146 (0.056)		1.7	2.1

The std. deviations  $\sigma a_i$  of the coeffs.  $a_i$  are given in parentheses  
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$ ;  $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$

$N$ , no. of direct exptl. values;  $n$ , no. of coeffs.  $a_i$

All direct exptl. values equally weighted

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