

SELECTED DATA ON MIXTURES  
INTERNATIONAL DATA SERIES\*  
3A. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3128

Compiled by Thermodynamics Research Center

Components:	1. Ethyl methanoate, $C_3H_6O_2$ [159-94-4] 2. Propanol, $C_3H_8O$ [67-63-2]
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
Methods:	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, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

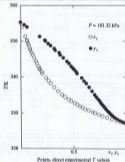
SOURCE OF DATA

See, A.; Hernández, F.; 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

$P/P_0 = 100.32$

$x_1$	$T/K$	$y_1$	$x_2$	$T/K$	$y_2$	$x_3$	$T/K$	$y_3$
0.000	395.39	0.000	0.204	541.80	0.336	0.775	329.26	0.874
0.010	394.63	0.056	0.242	539.77	0.380	0.820	328.81	0.884
0.017	394.07	0.061	0.263	538.88	0.402	0.866	328.35	0.917
0.045	391.35	0.141	0.285	538.20	0.623	0.911	327.92	0.941
0.060	390.28	0.200	0.317	537.17	0.649	0.950	327.59	0.964
0.082	390.05	0.256	0.353	536.30	0.677	0.938	327.37	0.982
0.070	349.35	0.282	0.385	335.17	0.701	1.000	327.29	1.000
0.077	348.77	0.284	0.420	336.49	0.718			
0.089	347.95	0.309	0.454	335.92	0.736			
0.095	347.51	0.328	0.478	335.39	0.751			
0.105	346.80	0.364	0.530	332.65	0.762			
0.113	346.17	0.376	0.539	332.40	0.775			
0.127	345.39	0.485	0.562	331.96	0.787			
0.144	344.41	0.438	0.584	331.61	0.799			
0.154	343.83	0.459	0.610	331.28	0.809			
0.168	343.05	0.479	0.643	330.80	0.820			
0.177	342.46	0.497	0.682	330.38	0.835			
0.182	342.17	0.506	0.705	330.00	0.845			
0.198	341.57	0.528	0.749	329.66	0.859			



Points, direct experimental  $T$  values.

AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 30 cm<sup>3</sup>, ref. 3. Turbidity ending of the phase enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and a Fischer model VE1 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  $\pm 0.01$  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 precision of  $\pm 0.02$  kg m<sup>-3</sup>. A polynomial equation describing density concentration curve obtained from mixtures of known composition was used in calculations. Estimated accuracy of composition  $>0.003$  mole fraction.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $\rho(298.15 \text{ K}) = 1.3176$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 914.93$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), purity  $>99.5$  mole %; degassed ultrasonically, dried over molecular sieves 3A;  $\rho(298.15 \text{ K}) = 1.3753$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 781.08$ , ref. 4.

$M(T)/K = 0.06$ ;  $10^5(P_0/P_0) = 30$ ;  $|\Delta x_1| = 0.002$ ;  $|\Delta y_1| = 0.005$ .

REFERENCES

- Int. Data Ser., Ser. A, *Goldberg J.*, 1994, 27(4).
- See, A.; Hernández, F.; Ortega, J. *Fluid Phase Equilib.*, 1998, 145, 311.
- Ortega, J.; Peña, J. A.; de Alencar, C. *J. Chem. Eng. Data*, 1996, 31, 339.
- Ortega, J.; Swaid, P. *J. Chem. Eng. Jpn.*, 1993, 26, 259.

**Components:** 1. Ethyl methacrylate,  $C_5H_8O_2$  /180-04-1/  
2. 2-Propanol,  $C_3H_8O$  /57-81-0/

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

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, de table 26: Universidad de Las Palmas de Gran Canaria, 35011 Las Palmas de Gran Canaria, Canary Islands, Spain)

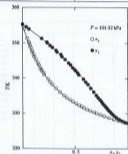
**Edited by:** Gross, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-003 Warszawa, Poland)

SOURCE OF DATA

Soto, A.; 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

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

P/Pa = 101.32		
$x_1$	T/K	$y_1$
0.00	355.39	0.0000
0.05	350.81	0.2091
0.10	347.08	0.3605
0.15	344.04	0.4540
0.20	341.34	0.5322
0.25	338.46	0.5925
0.30	335.72	0.6405
0.40	334.99	0.7117
0.50	332.96	0.7641
0.60	331.38	0.8087
0.70	328.08	0.8456
0.75	328.31	0.8653
0.80	328.96	0.8859
0.85	328.48	0.9084
0.90	328.03	0.9337
0.95	327.62	0.9635
1.00	327.29	1.0000



Points, direct experimental  $T$  values; circles,  $T(x_i)$  and  $T(y_i)$ , calculated from the equations.

**EQUATIONS**

$$G^E/RT = -x_1(a_1x_1 + a_2x_1^2) - x_2[a_3(x_1 + x_2)^2]$$

$$v_1 = \exp\left[-(a_1 + \frac{a_2}{T})x_1\right] \quad v_2 = \exp\left[-(a_3 + \frac{a_4}{T})x_2\right]$$

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

$$\mu_1^L = G^E - x_2(B_{12}^E / x_1 v_1) \quad \mu_2^L = G^E - x_1(B_{21}^E / x_2 v_2)$$

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

**COEFFICIENTS IN THE EQUATIONS**

P/Pa	$a_1$ /K	$a_2$ /K <sup>2</sup>	$a_3$ /K	$a_4$ /K <sup>2</sup>
101.32	254.25 16.31	0 108	89.725 14.50	0 100

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

P/Pa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	14.0056 (0.0008)	-2035.15 (0.0008)	-57.17 (0.0008)	16.67592 (0.0008)	-3646.20 (0.0008)	-53.54 (0.0008)

Standard deviation of  $T$ /K, relative standard deviation 100 $\sigma$ ( $T$ )/ $T$ , and absolute maximum deviation  $\delta$ ,  $\delta$ /K at P/Pa = 101.32 are resp. 0.008, 0.443, 0.327.

AUXILIARY INFORMATION

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

**Computations:** The 45  $T_{exp}$  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 relation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_{ii}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^L$ , ref. 6.

**Error:** Standard deviation  $\sigma(T) = [217 - T_{exp}]^2 / (N - 2)^{1/2}$   
Relative standard deviation 100 $\sigma$ ( $T$ )/ $T$  = 100[217 -  $T_{exp}$ ]/ $T_{exp}$   $\times$   $(N - 2)^{-1/2}$   
 $N$ , number of experimental points, ref. 2.  
 $a$ , number of coefficients in the smoothing equation.

REFERENCE

- Int. DATA Ser., Ser. A, *Chalidion*, Jan. 1995, 3(12).
- Ortega, J. *Int. DATA Ser., 2nd Data Volume, Ser. A*, 2001, 31, 69.
- Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 121.
- TRC Thermodynamic Tables - Hydrocarbons & Non-Hydrocarbons, 1988, 1-5728, 1988, 1-5018, Thermodynamics Research Center, The Texas A&M University System, College Station, TX, USA.
- Tsonopoulos, C. *AIChE J.*, 1974, 20, 263; 1975, 21, 821.
- Yan, L. C.; Woods, S. S. *AIChE J.*, 1964, 12, 95.

SELECTED DATA ON MIXTURES  
International Data Series\*  
No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3338

Compiled by Thermodynamic Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  (30-60-0)  
2. Ethyl ethanoate,  $C_4H_8O_2$  (10-20-6)

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

**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

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

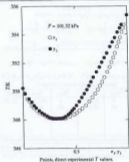
**Editor(s):** Skrzeci, A.; Majczak, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

Hernández, F.; 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

PMPa = 101.32									
$x_2$	PK	$y_2$	$x_2$	PK	$y_2$	$x_2$	$y_2$	PK	$y_2$
0.000	330.25	0.000	0.320	348.09	0.313	0.886	351.37	0.793	
0.026	349.85	0.022	0.545	348.30	0.390	0.829	351.71	0.732	
0.042	349.49	0.057	0.264	348.30	0.347	0.848	352.05	0.756	
0.066	348.27	0.083	0.280	348.11	0.358	0.866	352.37	0.780	
0.085	348.02	0.105	0.395	348.12	0.369	0.883	352.69	0.804	
0.103	348.46	0.125	0.408	348.14	0.379	0.903	353.15	0.835	
0.132	348.46	0.134	0.445	348.23	0.402	0.919	353.47	0.839	
0.157	348.51	0.178	0.484	348.37	0.428	0.933	353.78	0.882	
0.184	348.28	0.202	0.311	348.50	0.447	0.948	354.17	0.908	
0.211	348.28	0.226	0.536	348.65	0.464	0.962	354.47	0.930	
0.234	348.29	0.286	0.565	348.80	0.483	0.971	354.71	0.947	
0.253	348.34	0.282	0.599	349.02	0.508	1.000	355.39	1.000	
0.267	348.34	0.272	0.630	349.29	0.535				
0.270	348.15	0.275	0.661	349.58	0.560				
0.278	348.12	0.279	0.690	349.85	0.584				
0.278	348.11	0.280	0.714	350.12	0.609				
0.277	348.18	0.281	0.736	350.39	0.629				
0.289	348.09	0.289	0.757	350.67	0.649				
0.302	348.10	0.298	0.778	350.99	0.673				



AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass ebullometer 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 ebullometer was connected to a vacuum pump and the pressure controlled by a Vakuum electronic instrument (Normschilf Gerätebau Wertheim) and measured with a mercury manometer.

**Procedure:** The procedure was described in ref. 5. 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 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;  $\rho(298.15 \text{ K}) = 1.3752$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 790.77$ .

2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A;  $\rho(298.15 \text{ K}) = 1.3699$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 894.36$ .

**Errors:**  $|\Delta T/K| = 0.01$ ;  $|\Delta P/\text{Pa}| = 20$ ;  $|\Delta x_i| = 0.003$ ;  $|\Delta y_i| = 0.001$ .

REFERENCES

1. *Int. Data Ser., Ser. A, Guidelines*, 1994, 2114.
2. Hernández, F.; Ortega, J. *J. Chem. Eng. Data*, 1997, 42, 1399.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. *J. Chem. Eng. Data*, 1996, 41, 339.

Compiled by Thermodynamics Research Center

Components:	1. 2-Propanol, $C_3H_8O$ (50-63-0)
	2. Ethyl ethanoate, $C_4H_8O_2$ (101-79-0)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	$T$ , temperature $x_i$ , molar fraction of component $i$ in liquid phase $y_i$ , molar fraction of component $i$ in vapor phase
Parameters:	$P$ , pressure
Method:	Calculations 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 Filoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35091 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

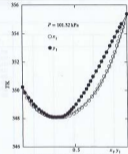
## SOURCE OF DATA

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

Note: The table reports unrounded values of  $T$  and calculated values of  $y_i$

PMPs = 101.32				
$x_1$	T/K	$y_1$		
0.00	330.25	0.0000		
0.05	349.45	0.0722		
0.10	348.87	0.1314		
0.15	348.49	0.1817		
0.20	348.25	0.2239		
0.25	348.11	0.2657		
0.30	348.06	0.3026		
0.40	348.17	0.3717		
0.50	348.52	0.4396		
0.60	348.12	0.5119		
0.70	356.01	0.5960		
0.75	350.58	0.6418		
0.80	351.26	0.6948		
0.85	352.86	0.7549		
0.90	353.80	0.8241		
0.95	354.10	0.9047		
1.00	353.79	1.0000		

Standard deviation  $\sigma(T)$ , relative standard deviation  $100\sigma(T)/T$ , and absolute maximum deviation  $\Delta_{max}(T)$  of PMPs = 101.32 are resp.: 0.053, 0.159, 0.092.



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

## EQUATIONS

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

$$v_1 = \exp \left[ -\left( A_{11} + \frac{A_{12}}{T} \right) / RT \right] \quad v_2 = \exp \left[ -\left( A_{22} + \frac{A_{21}}{T} \right) / RT \right]$$

$$P = P_1^* y_1 + P_2^* y_2 = \sum_{i=1}^2 x_i P_i^* \exp \left[ \frac{A_i^* (1-x_i) - P_i^* (1-x_i)^2}{RT} \right]$$

$$P_i^* = G_i^* - x_i (\Delta G_i^* / \Delta n_i)_{T,P} \quad A_i^* = G_i^* - x_i (\Delta G_i^* / \Delta n_i)_{T,P}$$

$$\Delta G_i^* = \Delta_i H_i^* - \Delta_i S_i^* T; \Delta_i S_i^* = R \ln(P_i^*/P); \quad P_i^*/P = \exp \{ A_i + B_i (C_i/T) + D_i \}$$

COEFFICIENTS IN THE EQUATIONS

PMPs	$A_i/K$	$B_i/K^2$	$C_i/K$	$D_i/K^2$
101.32	65.276 (4.2)	0 (0)	103.24 (4.9)	0 (0)

The standard deviations ( $\sigma_{A_i}$ ) of the coefficients  $A_i$  are given in parentheses.

PMPs	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	16.6792	-3640.20	-53.54	14.1265	-2311.89	-68.48

## AUXILIARY INFORMATION

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

Computations: The 50  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies,  $G_i^E$ .

Correlations: 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,  $V_i^L$ , ref. 6.

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

## REFERENCES

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- Ortega, J. *Int. Data Ser., Ser. A* (Data Volume, Ser. A) 2003, 31, 51.
- Wilson, G. M. *J. Am. Chem. Soc.* 1964, 86, 127.
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- Theodoropoulos, C. *AIChE J.* 1994, 30, 263; 1975, 21, 823.
- Yeo, L. C.; Woods, S. S. *AIChE J.* 1966, 12, 95.

SELECTED DATA ON MIXTURES  
International DATA Series\*  
A. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

Components	1, 2-Propanol, $C_3H_8O$ (67-63-0) 2-Propyl methanone, $C_6H_{12}O_2$ (739-74-7)
State	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables	$T$ , temperature $x_1$ , mole fraction of component 1 in liquid phase $y_1$ , mole fraction of component 1 in vapor phase $P$ , pressure
Parameters	$P_1^s$ , pure component 1 saturation pressure
Method	Direct measurement of $T$ , $x_1$ , and $y_1$ at constant $P_1^s$ (ref. 1)

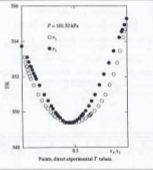
Author(s)	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Revised by	Shrock, A.; Marzylek, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 46/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

González, C.; Ortega, J.; Hernández, P.; Galindo, 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

$P/P_1^s = 101.32$									
$x_1$	TK	$y_1$	$x_1$	TK	$y_1$	$x_1$	TK	$y_1$	
0.000	353.75	0.000	0.402	348.43	0.413	0.871	352.16	0.718	
0.028	353.12	0.050	0.406	348.42	0.414	0.906	352.08	0.828	
0.054	352.85	0.066	0.412	348.41	0.437	0.936	352.07	0.874	
0.043	352.80	0.082	0.437	349.41	0.446	0.967	354.24	0.927	
0.049	352.59	0.087	0.442	349.41	0.463	0.979	354.57	0.951	
0.056	352.40	0.094	0.431	349.45	0.480	0.983	354.68	0.959	
0.063	352.21	0.110	0.359	349.47	0.499	0.992	354.96	0.979	
0.073	352.05	0.124	0.570	349.56	0.528	1.000	355.30	1.000	
0.085	351.89	0.136	0.602	349.66	0.542				
0.111	351.53	0.166	0.632	349.79	0.562				
0.154	351.00	0.251	0.638	349.80	0.567				
0.189	350.65	0.286	0.645	349.83	0.572				
0.221	350.35	0.276	0.648	349.87	0.574				
0.241	350.20	0.290	0.654	349.91	0.579				
0.273	349.99	0.305	0.685	350.00	0.602				
0.292	349.88	0.330	0.725	350.35	0.632				
0.308	349.78	0.342	0.735	350.64	0.658				
0.330	349.68	0.359	0.791	351.00	0.692				
0.365	349.53	0.388	0.833	351.55	0.735				



AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass ebullimeter 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 ebullimeter was connected to a vacuum pump and a Dumas-type of Hest model PPC2 pressure controller/calibrator with an uncertainty of ±0.02 kPa. The temperatures were measured by a digital thermometer Comark Electronics model 6009 with a PT-100 sensor. The thermometer was periodically calibrated with respect to the ITS-90 using a standard ASL-925 thermometer with the estimated uncertainty of the reading 0.02 °C.

**Procedure:** The procedure was described in ref. 3. The compositions were determined by measuring their densities at 296.15 K with an Anton Paar model DMA-55 vibrating-tube digital densimeter with a precision of ±0.02 kg m<sup>-3</sup>. A 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,  $\rho(296.15 \text{ K}) = 1.5752$ ,  $\rho(296.15 \text{ K})/\text{kg m}^{-3} = 761.33$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade, degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc,  $\rho(296.15 \text{ K}) = 1.3144$ ,  $\rho(296.15 \text{ K})/\text{kg m}^{-3} = 899.29$ .

**Errors:**  $|dT|_{\text{K}} = 0.02$ ,  $|dP|_{\text{kPa}} = 0.01$ ,  $|dx_1| = 0.002$ ,  $|dy_1| = 0.01$ .

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DOI: 10.1021/bk-2003-0113

53

Int. Data Ser., Ser. A, *Guldner*, 1994, 25(4)

**SELECTED DATA ON MIXTURES**  
**International Data Series\***  
**No. LIQUID-VAPOR EQUILIBRIUM**

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

**Components:** 1. 1-Propene,  $C_3H_6O$  [67-63-6]  
 2. Propyl methanoate,  $C_6H_{12}O_2$  [119-74-7]  
**State:** Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor  
**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase  
**Parameters:**  $P$ , pressure  
**Method:** 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, de la Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

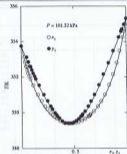
**Editor(s):** Chao, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

**SOURCE OF DATA**

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

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

P/Pa = 101.32						
$x_1$	T/K	$y_1$				
0.00	313.75	0.0000				
0.05	312.58	0.0025				
0.10	311.68	0.1511				
0.15	310.98	0.2097				
0.20	310.46	0.2607				
0.25	310.06	0.3039				
0.30	309.78	0.3498				
0.40	309.47	0.4195				
0.50	309.45	0.4854				
0.60	309.58	0.5303				
0.70	310.19	0.6202				
0.75	310.59	0.6397				
0.80	311.10	0.7043				
0.85	311.36	0.7562				
0.90	312.62	0.8188				
0.95	313.77	0.8934				
1.00	315.30	1.0000				



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

**EQUATIONS**

$$G^E/RT = -x_1(a_1 + a_2x_1) - x_2(a_2 + a_1x_2)$$

$$v_1 = \exp\left[-(a_1 + \frac{a_2}{T})x_1\right] \quad v_2 = \exp\left[-(a_2 + \frac{a_1}{T})x_2\right]$$

$$P = P_1^s - P_2^s - \sum_{i=1}^2 x_i P_i^s \exp\left[\frac{P_i^s (B_{1i} - 17)P - P_i^s - 2P B_{1i}^2 (1 - y_1)^2}{RT}\right]$$

$$P_i^s = G_i^s - a_i(G_i^s / (a_1)_{T,P}) \quad P_j^s = G_j^s - a_j(G_j^s / (a_2)_{T,P})$$

$$B_{1i}^2 = B_{1i} - (B_{1i} + B_{2i})x_2, y_1 = P/P^s; \quad P_i^s/P^s = \exp[A_i + B_i/T + C_i(T)]$$

**COEFFICIENTS IN THE EQUATIONS**

P/Pa	$a_1$ /K	$a_2$ /K <sup>2</sup>	$a_3$ /K	$a_4$ /K <sup>2</sup>
101.32	233.44 (6.4)	0 0.0	66.987 (3.3)	0 0.0

The standard deviations ( $\sigma_{a_j}$ ) of the coefficients  $a_j$  are given in parentheses.

P/Pa	$A_i$	$B_i$	$C_i$	$A_2$	$B_2$	$C_2$
101.32	16.8151	-3648.26	-13.54	15.77071	-3687.22	-69.07

Standard deviation  $\sigma(T)$ , relative standard deviation  $100(\Delta T/T)$ , and absolute standard deviation  $\sigma_a(T/K)$  at  $P/Pa = 101.32$  are resp.: 0.044, 0.159, 0.046.

**AUXILIARY INFORMATION**

**Measurements:** The  $T_{exp}$  data at 101.32 kPa are reported in ref. 2.  
**Computation:** The 46  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies,  $G^E$ .  
**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 imperfections and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_{1i}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^s$ , ref. 6.  
**Errors:** Standard deviation of  $T = [2(T - T_{exp})^2/(N-2)]^{1/2}$ .  
 Relative standard deviation  $100(\Delta T/T) = 100[2(T - T_{exp})^2/(N-2)]^{1/2}$ .  
 $N$ , number of experimental points, ref. 2.  
 $n$ , number of coefficients in the smoothing equation.

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JAN 2003 VOL 31 / NO 1

34

JAN 2003 VOL 31 / NO 1

Compiled by Thermodynamic Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  [57-65-8]  
2. Ethyl propanoate,  $C_5H_{10}O_2$  [105-37-1]

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

**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

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

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

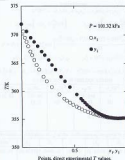
## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

 $P/P_a = 101.32$ 

$x_1$	$T/K$	$y_1$	$x_2$	$T/K$	$y_2$	$x_3$	$T/K$	$y_3$
0.000	371.52	0.000	0.544	357.30	0.656	0.876	355.28	0.882
0.035	370.65	0.049	0.572	356.84	0.674	0.885	355.27	0.889
0.034	369.35	0.089	0.600	356.59	0.693	0.895	355.26	0.898
0.049	368.83	0.122	0.629	356.37	0.700	0.905	355.25	0.905
0.065	368.06	0.153	0.656	356.20	0.727	0.920	355.24	0.910
0.084	367.10	0.193	0.678	356.05	0.742	0.913	355.24	0.913
0.104	366.47	0.222	0.702	355.92	0.756	0.922	355.24	0.921
0.122	365.62	0.258	0.714	355.85	0.764	0.929	355.25	0.927
0.143	364.73	0.289	0.731	355.75	0.776	0.941	355.26	0.938
0.168	363.93	0.323	0.748	355.68	0.787	0.931	355.27	0.944
0.208	362.63	0.375	0.772	355.57	0.803	0.963	355.28	0.961
0.230	361.94	0.412	0.789	355.52	0.815	0.976	355.29	0.973
0.286	360.80	0.459	0.803	355.46	0.825	1.008	355.30	1.000
0.339	359.69	0.525	0.814	355.42	0.830			
0.405	358.76	0.564	0.823	355.39	0.848			
0.428	358.42	0.580	0.836	355.37	0.858			
0.458	358.05	0.602	0.848	355.35	0.857			
0.489	357.67	0.620	0.855	355.32	0.865			
0.521	357.33	0.642	0.867	355.30	0.874			

Points, direct experimental  $T$  values.

## AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass-thermometer 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 stillonometer was connected to a vacuum pump and the pressure controlled by a Vakuumat electronic instrument (Stoesschli-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 208.15 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 polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty of composition  $\leq 0.003$  mole fraction.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieve 3A;  $n_D(20, 15 \text{ K}) = 1.3752$ ,  $\rho(208.15 \text{ K})/\text{kg m}^{-3} = 780.77$ .  
2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieve 3A;  $n_D(20, 15 \text{ K}) = 1.3811$ ,  $\rho(208.15 \text{ K})/\text{kg m}^{-3} = 883.93$ .

**Error:**  $|T/K - 0.01|$ ;  $|x_1/P_a - 10|$ ;  $|x_2| = 0.002$ ;  $|y_1| = 0.01$ .

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- Ortega, J.; Peña, J. A.; de Alencastro, C. *J. Chem. Eng. Data*, 1986, 31, 339.

SELECTED DATA ON MIXTURES  
International Data Series\*  
No. LIQ-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80505-3326

Compiled by Thermodynamic Research Center

**Compositor:** 1. 2-Propanol,  $C_3H_8O$  (67-63-0)  
2. Ethyl propionate,  $C_5H_{10}O_2$  (101-17-3)  
**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  
 $P$ , pressure  
**Method:** Calculation from direct experimental liquid-vapor equilibrium temperatures,  $T_{exp}$  data at variable  $x_i$  and constant  $P$ , ref. 1

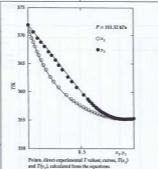
**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, de Icaña 36; Universidad de Las Palmas de Gran Canaria, 35011 Las Palmas de Gran Canaria, Canary Islands, Spain)  
**Editor(s):** Craya, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Herrández, F.; 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

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

P/Pa = 101.32		
$x_1$	T/K	$y_1$
0.00	371.97	0.0000
0.05	368.84	0.1323
0.10	366.43	0.2385
0.15	364.56	0.3161
0.20	362.93	0.3895
0.25	361.61	0.4566
0.30	360.52	0.5152
0.40	358.80	0.5699
0.50	357.54	0.6158
0.60	356.60	0.6585
0.70	355.92	0.7082
0.75	355.67	0.7522
0.80	355.47	0.8260
0.85	355.33	0.8624
0.90	355.27	0.9025
0.95	355.28	0.9477
1.00	355.39	1.0000



**EQUATIONS**

$$G^E/RT = -x_1(a_1 + x_2a_2) - x_2(b_1x_1 + x_2)$$

$$v_1 = \exp\left[-(a_1 + \frac{a_2}{x_1})/T\right] \quad v_2 = \exp\left[-(a_2 + \frac{a_1}{x_2})/T\right]$$

$$P = P_1^s + P_2^s - \sum_{i=1}^2 x_i^2 P_i^s \exp\left[\frac{A_i^s - (B_i^s - 17^2)(P - P_i^s) - 22B_i^s(1 - P_i^s)^2}{RT}\right]$$

$$\mu_i^s = G^s - x_i(RT^s / v_i^s)_{T,P} \quad \mu_i^l = G^l - x_i(RT^l / v_i^l)_{T,P}$$

$$B_{12}^s = B_{11} - (B_{11} + A_{22})/2; \gamma_1 = P_1/P; \quad P_i^s/\text{kPa} = \exp\{4.4 + B_i/(C_i + T/K)\}$$

**COEFFICIENTS IN THE EQUATIONS**

P/Pa	$a_1$ /K	$a_2$ /K <sup>2</sup>	$a_3$ /K	$a_4$ /K <sup>2</sup>
101.32	185.46	0	50.849	0
	(3.5)	(0)	(2.8)	(0)

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

P/Pa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	16.47792	-1649.20	-53.54	14.15418	-2393.11	-64.15

Standard deviations of  $T$ , K, relative standard deviation 300 $\sigma$ ( $\sigma$ )/ $T$ , and absolute maximum deviation  $\delta_{max}$  T/K at P/Pa = 101.32 are resp.: 0.040, 0.130, 0.184.

**AUXILIARY INFORMATION**  
**Measurements:** The  $T_{exp}$  data at 101.32 kPa are reported in ref. 2.  
**Computations:** The 31  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $\mu_i^E$ .  
**Comments:** 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  $B_{ii}$ , ref. 5, and the molar volumes under saturation pressure  $V_{i,s}^L$ , ref. 6.  
**Errors:** Standard deviation of  $T$  =  $\sum(T - T_{exp})^2/(N-2)^{1/2}$ .  
Relative standard deviation 100 $\sigma$ ( $\sigma$ )/ $T$  =  $100\sum(T - T_{exp})^2/P_{exp}^2/(N-2)^{1/2}$ .  
 $N$ , number of experimental points, ref. 2.  
 $n$ , number of coefficients in the smoothing equation.

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DATE RECEIVED: 01/01/03

58

JULY 2003 VOL. 31, NO. 14



Compiled by Thermodynamic Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  (302-63-0)  
2. Propyl ethanoate,  $C_5H_{10}O_2$  (109-60-0)

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

**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P_i^s$ , pressure

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

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

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

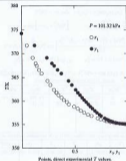
## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

P/P<sub>1</sub> = 308.32

$x_1$	$T/K$	$y_1$	$x_1$	$T/K$	$y_1$	$x_1$	$T/K$	$y_1$
0.000	334.31	0.000	0.599	337.95	0.693	0.991	355.20	0.989
0.049	331.36	0.123	0.590	337.55	0.715	0.993	355.20	0.993
0.105	309.35	0.240	0.626	337.14	0.737	1.000	355.20	1.000
0.132	308.00	0.287	0.600	336.85	0.753			
0.145	307.47	0.309	0.719	336.40	0.786			
0.164	306.62	0.342	0.747	336.16	0.805			
0.189	305.87	0.377	0.781	336.00	0.822			
0.245	304.30	0.444	0.802	335.79	0.837			
0.270	303.45	0.476	0.808	335.88	0.841			
0.304	302.43	0.511	0.835	335.66	0.860			
0.328	301.81	0.535	0.849	335.68	0.865			
0.330	301.81	0.531	0.876	335.46	0.891			
0.348	301.28	0.552	0.899	335.08	0.906			
0.377	300.75	0.573	0.928	335.30	0.931			
0.398	300.27	0.596	0.950	335.25	0.932			
0.428	339.80	0.618	0.964	335.23	0.963			
0.445	339.33	0.638	0.973	335.21	0.974			
0.496	338.86	0.658	0.981	335.20	0.979			
0.529	338.43	0.669	0.986	335.20	0.984			

Points, direct experimental  $T$  values.

## AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass ebullimeter employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm<sup>3</sup>, ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebullimeter was connected to a vacuum pump and a Desgrippes et Haut model PPC2 pressure controller/calibrator with an uncertainty of  $\pm 0.02$  kPa. The temperatures were measured by a digital thermometer Comark Electronics model 6808 with a PT-300 sensor. The thermometer was periodically calibrated with respect to the ITS-90 using a standard ASL-825 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-35 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  $g/g$ ;  $\rho(298.15 \text{ K}) = 1.3752$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 761.30$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by  $g/g$ ;  $\rho(298.15 \text{ K}) = 1.2016$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 682.63$ .

**Error:**  $|dP/P| = 0.05$ ;  $|dy_1/y_1| = 2\%$ ;  $|dx_1/x_1| = 0.003$ ;  $|dy_2/y_2| = 0.01$ .

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2. González, C.; Ortega, J.; Hernández, P.; Gubón, S. *J. Chem. Eng. Data*, 1999, 44, 732.
3. Ortega, J.; Peña, J. A.; de Alfonso, C. *J. Chem. Eng. Data*, 1996, 41, 939.

SELECTED DATA ON MIXTURES  
International Data Series<sup>®</sup>  
No. LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamic Research Group

National Institute of Standards and Technology, Boulder, CO 80505-3328

**Components:** 1. 2-Propanol,  $C_3H_8O$  (67-63-6)  
2. Propyl ethanoate,  $C_5H_{10}O_2$  (109-66-4)

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

**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase

**Parameters:**  $P$ , pressure

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

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, s/n de la Universidad de Las Palmas de Gran Canaria, 36070 Las Palmas de Gran Canaria, Canary Islands, Spain)

**Edited by:** Onda, F. (Wydział Chemii, Uniwersytet Warszawski, al. Pasteura 1, 02-093 Warszawa, Poland)

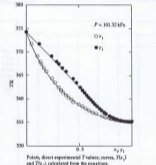
SOURCE OF DATA

González, C.; Ortega, J.; Hernández, P.; Colino, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), FIRST PUBLISHED 1995(1), 19

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

PMPa = 101.32					
$x_1$	T/K	$y_1$			
0.00	374.34	0.0000			
0.05	371.49	0.1255			
0.10	369.15	0.2271			
0.15	367.15	0.3418			
0.20	365.40	0.5037			
0.25	363.90	0.6458			
0.30	362.59	0.8002			
0.40	360.43	0.9117			
0.50	358.76	0.9668			
0.60	357.46	0.9744			
0.70	356.48	0.9760			
0.75	356.09	0.9786			
0.80	355.77	0.9876			
0.85	355.51	0.9932			
0.90	355.33	0.9919			
0.95	355.24	0.9910			
1.00	355.38	1.0000			

Standard deviation of  $T$  (K), relative standard deviation 100( $\Delta T$ )/ $T$ , and absolute maximum deviation  $d_{max}$  (K) at PMPa = 101.32 are resp. 0.113, 0.410, 0.287.



**EQUATIONS**

$$G^E/RT = -a_1(x_1 + c_1x_1^2) - a_2(x_1^2 + c_2x_1^3)$$

$$v_1 = \exp\left[-b_1 + \frac{c_1^2}{2}x_1^2\right] \quad v_2 = \exp\left[-b_2 + \frac{c_2^2}{2}x_2^2\right]$$

$$P = P_1^s + P_2^s - \sum_{i=1}^2 v_i^2 \exp\left[\frac{v_i^E - (R_{11} - v_i^2)(P - P_i^s) - 2Pv_i^E(1 - y_i)^2}{RT}\right]$$

$$v_i^E = G^E - a_i(40^\circ C / dx_i)_{220} \quad v_i^s = G^E - a_i(40^\circ C / dx_i)_{220}$$

$R_1^E = R_{1,1} - (R_{1,1} + R_{2,2})/2 - v_1^E - P_i^s/P$ ;  $P_i^s$  (kPa) =  $\exp[A_i + B_i/(C_i + T/K)]$

**COEFFICIENTS IN THE EQUATIONS**

PMPa	$a_1$ /K	$a_2$ /K <sup>2</sup>	$a_3$ /K	$a_4$ /K <sup>2</sup>
101.32	379.11	0	-104.72	6
	(0.15)	(0)	(7.20)	(0)

The standard deviations ( $\Delta a_j$ ) of the coefficients  $a_j$  are given in parentheses.

PMPa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	16.6810	-3640.20	-53.34	13.9331	-2840.15	-30.67

**AUXILIARY INFORMATION**

**Measurements:** The  $T_{exp}$  data at 101.32 kPa are reported in ref. 1.

**Computation:** The 41  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies,  $v_i^E$ .

**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 imperfections and the variation of the Gibbs energy of the pure liquid component with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_{ii}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^s$ , ref. 6.

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

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10.1066/10000001-1010

38

Int. Data Ser., Ser. A, *Collected Vol.*, 2003, 31, 03, 40-72

SELECTED DATA ON MIXTURES  
International Data Series\*  
26. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80501-3328

Compiled by Thermodynamics Research Center

Component:	1. 2-Propanol, $C_3H_8O$ [67-63-0] 2. Ethyl acetate, $C_4H_8O_2$ [105-54-4]
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variable:	$T$ , temperature $x_i$ , mole fraction of component $i$ in liquid phase $y_i$ , mole fraction of component $i$ in vapor phase
Parameter:	$P$ , pressure
Method:	Direct measurement of $T$ , $x_i$ and $y_i$ at constant $P$ , ref. 1

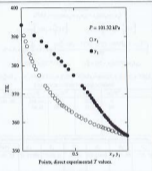
Author(s) of table:	Ortega, J. (Laboratorio de Termodinámica y Psicrometría, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by:	Slawski, A., Majczyk, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 64/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

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

DIRECT EXPERIMENTAL VALUES

$P/101.32$									
$x_2$	$T/K$	$y_2$	$x_2$	$T/K$	$y_2$	$x_2$	$T/K$	$y_2$	
0.000	394.38	0.000	0.420	365.22	0.732	0.925	356.26	0.960	
0.021	390.57	0.122	0.464	364.55	0.745	0.929	356.21	0.962	
0.038	388.50	0.190	0.472	363.85	0.759	0.931	355.92	0.974	
0.051	386.80	0.237	0.505	362.78	0.782	0.932	355.92	0.975	
0.074	384.33	0.326	0.543	362.18	0.793	0.932	355.79	0.985	
0.088	382.60	0.548	0.565	361.63	0.807	0.934	355.67	0.986	
0.101	381.50	0.578	0.603	361.08	0.821	1.000	355.39	1.000	
0.119	379.95	0.615	0.647	360.18	0.838				
0.133	378.75	0.644	0.687	359.40	0.855				
0.165	376.65	0.695	0.726	358.30	0.872				
0.225	373.00	0.578	0.754	358.51	0.883				
0.240	372.10	0.594	0.778	358.20	0.890				
0.258	370.70	0.628	0.791	357.93	0.900				
0.291	369.70	0.647	0.817	357.59	0.911				
0.313	368.70	0.664	0.825	357.54	0.914				
0.337	367.85	0.682	0.854	357.88	0.928				
0.355	367.13	0.694	0.858	357.85	0.931				
0.376	366.27	0.710	0.892	356.85	0.943				
0.392	365.98	0.716	0.894	356.61	0.945				



AUXILIARY INFORMATION

Apparatus:	The apparatus was a glass ebullioscope 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 ebullioscope was connected to a vacuum pump and the pressure controlled by a Yokumata electronic instrument (Normachill Gerüchbau Wetzlar) and measured with a mercury manometer.
Procedure:	The procedure was described in ref. 3. The compositions were determined by measuring their densities at 296.15 K with an Anton Paar model DMA-35 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; $\rho(296.15 \text{ K}) = 1.3753$ , $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 780.77$ . 2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; $\rho(296.15 \text{ K}) = 1.3096$ , $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.94$ .
Errors:	$ u(T)  < 0.05$ ; $ u(P)  < 10$ ; $ u(x_i)  = 0.002$ ; $ u(y_i)  = 0.01$ .

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- Hernández, F., Ortega, J. *J. Chem. Eng. Data*, 1997, 42, 1690.
- Ortega, J., Peña, I. A., de Alkous, C. *J. Chem. Eng. Data*, 1986, 31, 130.

SELECTION DATA ON MIXTURES  
International Data Series\*  
No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Boulder, CO 80501-3328

Compiled by Thermodynamic Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  (67-63-0)  
2. Ethyl acetate,  $C_4H_8O_2$  (101-54-4)  
**State:** Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor  
**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase  
 $P$ , pressure  
**Method:** Calculated 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, Universidad de Las Palmas de Gran Canaria, 35011 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

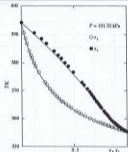
SOURCE OF DATA

Herráiz, F.; 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  $y_i$ .

Pb/Pa = 101.32		
$x_1$	T/K	$y_1$
0.00	304.18	0.0000
0.05	306.84	0.2152
0.10	308.54	0.3561
0.15	307.67	0.4567
0.20	304.23	0.5328
0.25	301.56	0.5928
0.30	300.32	0.6407
0.40	305.76	0.7177
0.50	305.89	0.7755
0.60	300.86	0.8229
0.70	309.25	0.8648
0.75	308.49	0.8890
0.80	307.79	0.9052
0.85	307.14	0.9261
0.90	306.52	0.9482
0.95	305.94	0.9725
1.00	305.30	1.0000

Standard deviation  $\sigma(T)$ , K, relative standard deviation  $100\sigma(T)/T$ , and absolute maximum deviation  $\delta_{max}(T)$ , K at Pb/Pa = 101.32 are resp.: 0.075, 0.242, 0.200.



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

**EQUATIONS**

$$G^E(2T) = -x_1 \ln(x_1 + \alpha_1 x_1^2) - x_2 \ln(x_2 + \alpha_2 x_2^2)$$

$$\alpha_1 = \exp\left[-(a_1 + \frac{b_1}{T})/T\right] \quad \alpha_2 = \exp\left[-(a_2 + \frac{b_2}{T})/T\right]$$

$$P = P_1^s + P_2^s - \sum_{i=1}^2 \alpha_i P_i^s \exp\left[\frac{V_i^s - (V_i^s - V_i^l)P_i^s - P_i^s}{RT}\right]$$

$$P_i^s = G^s - \alpha_i (dG^s/dx_i)_{T,P} \quad P_i^l = G^l - \alpha_i (dG^l/dx_i)_{T,P}$$

$$H_{12}^E = H_{12}^E - (H_{11}^E + H_{22}^E)/2 - T \cdot \gamma; \quad P_i^s(Pa) = \exp\{A_i + B_i/(C_i + T)\}$$

**COEFFICIENTS IN THE EQUATIONS**

Pb/Pa	$a_1$ , K	$a_2$ , K <sup>2</sup>	$a_3$ , K	$a_4$ , K <sup>2</sup>
101.32	264.66	0	-33.016	0
	0.43	00	(4.30)	00

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

Pb/Pa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	36.6792	-3640.30	-53.54	12.1018	-2121.97	-112.77

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

**Computations:** The 45  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $G_i^E$ .

**Conventions:** 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  $B_{ii}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^s$ , ref. 6.

**Notes:** Standard deviation  $\sigma(T) = [2(T - T_{exp})^2]/N = 2(1)^2$   
Relative standard deviation  $100\sigma(T)/T = 100(10^{-2})/300 = 0.33\%$   
 $N$ , number of experimental points, ref. 2.  
 $\alpha_i$ , number of coefficients in the smoothing equation.

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0014-1801/03/010001-12\$15.00

60

Int. Data Ser., Ser. A, October 1991, 2(2)

Compiled by Thermodynamics Research Center

**Components:** 1. 1-Propanol,  $C_3H_7O$  (67-63-0)  
2. Propyl propanoate,  $C_6H_{12}O_2$  (706-36-3)

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

**Variables:**  $T$ , temperature  
 $x_1$ , mole fraction of component 1 in liquid phase  
 $y_1$ , mole fraction of component 1 in vapor phase

**Parameters:**  $P$ , pressure

**Method:** Direct measurement of  $T$ ,  $x_1$  and  $y_1$  at constant  $P$ ; ref. 1

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Piroquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 3501 Las Palmas de Gran Canaria, Canary Islands, Spain)

**Edited by:** Skrzyszewski, A.; Mroczek, A.; Gajda, J. (Instytut Fizyczny, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

## SOURCE OF DATA

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

## DIRECT EXPERIMENTAL VALUES

P/Pa = 101.32

$x_1$	TK	$y_1$	$x_2$	TK	$y_2$
0.000	395.56	0.000	0.896	356.58	0.942
0.028	392.00	0.112	0.926	356.29	0.956
0.035	390.95	0.141	0.955	355.82	0.970
0.047	387.43	0.248	0.968	355.76	0.980
0.144	388.05	0.439	0.974	355.61	0.979
0.235	373.80	0.585	0.984	355.57	0.988
0.281	371.06	0.645	0.985	355.55	0.985
0.381	366.92	0.718	0.995	355.55	0.995
0.453	364.76	0.755	0.995	355.55	0.995
0.510	363.30	0.783	0.999	355.54	0.999
0.580	361.90	0.812	0.999	355.53	0.999
0.659	360.68	0.859	0.994	355.53	0.994
0.717	359.37	0.869	0.995	355.53	0.994
0.751	358.81	0.887	0.995	355.53	0.994
0.794	358.19	0.903	0.995	355.52	0.994
0.828	357.53	0.922	1.000	355.50	1.000
0.864	357.34	0.950			
0.887	356.87	0.961			
0.891	356.68	0.964			

## AUXILIARY INFORMATION

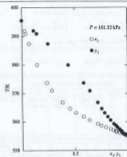
**Apparatus:** The apparatus was a glass ebullimeter employing continuous circulation of the liquid and vapor phases with a charge capacity of 30 cm<sup>3</sup>, vol. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebullimeter was connected to a vacuum pump and a Dwygintec oil-flood model PFC2 pressure controller/calibrator with an uncertainty of  $\pm 0.02$  kPa. The temperatures were measured by a digital thermometer Comack Electronics model 6800 with a PT-306 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 K.

**Procedure:** The procedure was described in ref. 3. The composition was determined by measuring their densities at 298.15 K with an Anton Paar model DMA 51 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 AD (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried in diasthen over molecular sieves 3A; no significant impurities by glc;  $\rho(0, 298.15 \text{ K}) = 1.3752, \rho(298.15 \text{ K})_{\text{glc}} = 781.33$ .

2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in diasthen over molecular sieves 3A; no significant impurities by glc;  $\rho(0, 298.15 \text{ K}) = 1.3908, \rho(298.15 \text{ K})_{\text{glc}} = 875.61$ .

**Errors:**  $\pm 0.10 \text{ K}$  in  $T$ ;  $\pm 0.01$  in  $x_1$ ;  $\pm 0.005$  in  $y_1$ ;  $\pm 0.01$ .

Points, direct experimental  $T$  values.

## REFERENCES

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- González, C.; Ortega, J.; Hernández, P.; Galán, S. *J. Chem. Eng. Data*, 1999, 44, 772.
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**SELECTED DATA ON MIXTURES**  
**International Data Series\***  
**No. LIQUID-VAPOR EQUILIBRIUM**

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  [57-05-0]  
 2. Propyl propanoate,  $C_6H_{12}O_2$  [100-36-3]  
**State:** Binary system, single phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor  
**Variables:**  $T$ , temperature  
 $x_i$ , mole fraction of component  $i$  in liquid phase  
 $y_i$ , mole fraction of component  $i$  in vapor phase  
**Parameters:**  $P$ , pressure  
**Method:** Calculation from direct experimental liquid-vapor equilibrium temperature,  $T_{exp}$ , data at variable  $x_i$  and constant  $P$ , ref. 1

**Author(s):** Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, deable 36, Universidad de Las Palmas de Gran Canaria, 2001 Las Palmas de Gran Canaria, Canary Islands, Spain)

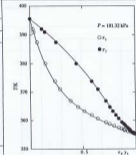
**Edited by:** Gross, F. (Wydział Chemii, Uniwersytet Warszawski, al. Pasteura 1, 02-093 Warszawa, Poland)

**SOURCE OF DATA**

González, C.; Ortega, J.; Hernández, F.; Ovelo, 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  $y_i$

PMPs = 101.32					
$x_1$	T/K	$y_1$			
0.00	305.56	0.0000			
0.05	309.34	0.2036			
0.10	303.91	0.3515			
0.15	319.42	0.4662			
0.20	315.75	0.5477			
0.25	312.76	0.6094			
0.30	318.30	0.6577			
0.40	306.50	0.7295			
0.50	303.67	0.7827			
0.60	301.43	0.8269			
0.70	306.58	0.8672			
0.75	308.75	0.8871			
0.80	307.86	0.9034			
0.85	307.25	0.9203			
0.90	306.56	0.9356			
0.95	303.91	0.9742			
1.00	305.30	1.0000			



Standard deviation  $\sigma(T)$ ,  $K$ , relative standard deviation 100 $\sigma(T)/T$ , and absolute maximum deviation  $\delta_{max}(T)$ ,  $K$ , at PMPs = 101.32 are resp.: 0.089, 0.325, 0.177.

**EQUATIONS**

$$G^E RT = -a_1 x_1 + a_2 x_1^2 - a_3 x_1^3 + c_1 x_1^4$$

$$c_1 = \exp\left[-b_1 + \frac{a_1}{RT}\right] \quad c_2 = \exp\left[-b_2 + \frac{a_2}{RT}\right]$$

$$P = P_1^s y_1 + \sum_{i=1}^2 P_i^s y_i^2 \exp\left[\frac{V_i^L (P - P_i^s) - 2P_i^s V_i^L (1 - y_i)^2}{RT}\right]$$

$$P_i^s = G^E - x_i^2 (RT^2 / \Delta x_i)_{T,P} \quad P_i^s = G^E - x_i (RT^2 / \Delta x_i)_{T,P}$$

**COEFFICIENTS IN THE EQUATIONS**

PMPs	$a_1/K$	$a_2/K^2$	$a_3/K$	$c_1/K^2$
101.32	-180.87 (151.8)	701344 (62941)	200.34 (42.8)	0 100

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

PMPs	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	15.68151	-3640.29	-35.34	14.81047	-3518.18	-47.83

**AUXILIARY INFORMATION**

**Measurements:** The  $T_{exp}$  data at 101.32 kPa are reported in ref. 2.  
**Computations:** The 35  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies  $G_i^E$ .  
**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  $V_i^s$ , ref. 6.  
**Errors:** Standard deviation  $\sigma(T) = [2(T - T_{exp})^2 / (N - 2)]^{1/2}$   
 Relative standard deviation 100 $\sigma(T)/T = 100[2(T - T_{exp})^2 / (N - 2)]^{1/2}$   
 $N$ , number of experimental points, ref. 2.  
 $n$ , number of coefficients in the smoothing equation.

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0014-1855/03/040001-12\$18

12

Int. Data Ser., Ser. Data Memores, Ser. A, 2003, 11(1), 01-12

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

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

**Components:** 1. *n*-Propanol, C<sub>3</sub>H<sub>8</sub>O (67-63-0)  
2. Propyl bromide, C<sub>3</sub>H<sub>7</sub>Br (105-69-5)

**Status:** 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):** 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)

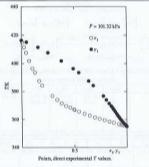
**Edited by:** Skrzeczo, A.; Muzyczak, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

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

DIRECT EXPERIMENTAL VALUES

<i>P</i> /kPa = 101.32						
<i>x<sub>1</sub></i>	<i>T</i> /K	<i>y<sub>1</sub></i>	<i>x<sub>2</sub></i>	<i>T</i> /K	<i>y<sub>2</sub></i>	
0.000	416.57	0.008	0.646	363.80	0.816	
0.007	415.30	0.048	0.695	361.73	0.827	
0.024	411.60	0.158	0.790	360.68	0.937	
0.043	407.70	0.253	0.788	359.74	0.968	
0.073	401.90	0.380	0.834	358.78	0.959	
0.103	396.45	0.492	0.875	357.84	0.968	
0.127	393.55	0.545	0.925	356.95	0.980	
0.168	387.65	0.639	0.945	356.47	0.986	
0.196	384.45	0.681	0.965	356.14	0.990	
0.205	376.91	0.779	0.981	355.81	0.995	
0.336	374.25	0.866	1.000	355.50	1.000	
0.380	371.79	0.932				
0.422	369.85	0.952				
0.464	368.68	0.964				
0.498	367.34	0.976				
0.500	367.15	0.978				
0.545	365.78	0.990				
0.597	364.36	0.905				



AUXILIARY INFORMATION

**Apparatus:** The apparatus was a glass ebullioscope 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 ebullioscope was connected to a vacuum pump and a Dwygans et al. model PFC2 pressure controller/calibrator with an uncertainty of ±0.02 kPa. The temperatures were measured by a digital thermometer Comark Electronics model 6800 with a PT-300 sensor. The thermometer was periodically calibrated with respect to the ITS-90 using a standard ASL-735 thermometer with the estimated uncertainty of the reading 0.02 °C.

**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 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 ethanically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $\rho(0.1, 298.15 \text{ K}) = 1.3752, \rho(0.9, 298.15 \text{ K}) = 1.3833$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ethanically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $\rho(0.1, 298.15 \text{ K}) = 1.2975, \rho(0.9, 298.15 \text{ K}) = 1.3040$ .

**Notes:** |kT/K = 0.01; |kPa/0.1 = 20; |*x<sub>1</sub>*| = 0.0015; |*y<sub>1</sub>*| = 0.01.

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3. Ortega, J.; Peña, J. A.; de Alencastro, C. *J. Chem. Eng. Data, 1996, 31, 309.*

**SELECTED DATA ON MIXTURE\***  
**International Data Series\***  
**3a. LIQUID-VAPOR EQUILIBRIUM**

National Institute of Standards and Technology, Boulder, CO 80505-3332

Compiled by Thermodynamics Research Center

**Composition:** 1. 2-Propanol,  $C_3H_8O$  (67-63-0)  
 2. Propyl acetate,  $C_5H_{10}O_2$  (109-66-0)  
**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, Universidad de Las Palmas de Gran Canaria, 35015 Las Palmas de Gran Canaria, Canary Islands, Spain)

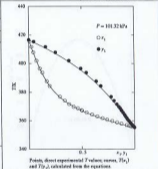
**Edited by:** Chua, F. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

**SOURCE OF DATA**

González, C.; Ortega, J.; Hernández, P.; Galisteo, 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  $y_i$ .

		P/Pa = 101.32				
$x_1$	TK	$y_1$				
0.00	416.57	0.0000				
0.05	406.37	0.2687				
0.10	393.26	0.6611				
0.15	380.87	0.9372				
0.20	384.22	0.6763				
0.25	379.83	0.7256				
0.30	376.33	0.7693				
0.40	371.09	0.8268				
0.50	367.23	0.8664				
0.60	364.17	0.8975				
0.70	361.59	0.9245				
0.75	360.42	0.9369				
0.80	359.32	0.9492				
0.85	358.26	0.9616				
0.90	357.24	0.9740				
0.95	356.26	0.9866				
1.00	355.30	1.0000				



**EQUATIONS**

$$G^E(T) = -x_1 \ln \gamma_1 + x_2 \ln \gamma_2 - x_1 x_2 (v_1 + v_2) \tau_{12}$$

$$\tau_{12} = \exp \left[ -A_{12} + \frac{B_{12}}{T} \right] \quad \tau_{21} = \exp \left[ -A_{21} + \frac{B_{21}}{T} \right]$$

$$P = P_1 + P_2 - \sum_{i=1}^2 x_i P_i^s \exp \left[ \frac{V_i^L (P - P_i^s) (1 - \gamma_i)^2}{RT} \right]$$

$$\ln \gamma_i^L = G^E - x_j (v_j^L / v_i^L) \tau_{ij} \quad \ln \gamma_j^L = G^E - x_i (v_i^L / v_j^L) \tau_{ij}$$

$$B_{12}^s = B_{12} - (B_{11} + B_{22})/2, \quad \gamma_i^s / P_i^s = \exp [A_i + B_i / (C_i + T)]$$

**COEFFICIENTS IN THE EQUATIONS**

P/Pa	$a_1$ /K	$a_2$ /K <sup>2</sup>	$a_3$ /K	$a_4$ /K <sup>2</sup>
101.32	-3577.14 (109.4)	675129 (32884)	304.79 (49.4)	0 00

The standard deviations ( $\sigma_{e_j}$ ) of the coefficients  $e_j$  are given in parentheses.

P/Pa	$A_1$	$B_1$	$C_1$	$A_2$	$B_2$	$C_2$
101.32	36.6816 (0.0011)	-3640.20 (30.54)	-53.54 (15.4263)	-2347.66 (2347.66)	-116.35 (116.35)	

Standard deviation of  $T$  (TK), relative standard deviation (100 $\Delta T/T$ ), and absolute maximum deviation  $\Delta_{max}(T/K)$  at P/Pa = 101.32 are resp.: 0.159, 0.157, 0.410.

**AUXILIARY INFORMATION**

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

**Computations:** The 29  $T_{exp}$  data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies,  $G_i^E$ .

**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 imperfections and the variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the 2nd molar virial coefficients  $B_{ii}$ , ref. 5, and the molar volumes under saturation pressure  $V_i^s$ , ref. 6.

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

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0010-236X/03/31(01)0010-10

10

Int. Data Ser., Ser. A, Vol. 31, No. 1, 2003, pp. 10-22



BIPHY-BIPACRYL-DMF

Compiled by Thermodynamics Research Center

Component: 1. Ethyl methacrylate,  $C_5H_8O_2$  [709-94-4]  
 2. Propagol,  $C_{12}H_{22}O$  [67-63-0]  
 State: Binary system, single phase liquid, pure components, both liquid  
 Variables:  $v^E$ , molar excess volume  
 $x_1$ , mole fraction of component 1  
 Parameters:  $T$ , temperature  
 Constants:  $P$ , pressure  
 Method: Calculation of  $V^E$  from density measurements of constant  $T$  and  $P$  and variable  $x_1$ , ref. 1

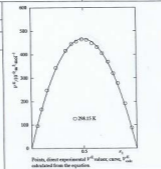
Author(s) Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)  
 Editor(s) Skrzacz, A.; Mącznyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk,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

SOURCE OF DATA  
 Note, A.; 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

TK = 298.15						
$x_1$	$v^E/10^{-6}$ $m^3 \cdot mol^{-1}$					
0.0565	76					
0.0964	157					
0.1505	268					
0.2378	344					
0.3328	417					
0.3878	445					
0.4350	455					
0.4882	465					
0.5329	463					
0.5828	448					
0.6322	432					
0.6783	406					
0.7341	369					
0.7814	320					
0.8239	278					
0.8912	191					
0.9320	88					



**SMOOTHING EQUATION**

$$v^E_{calc} = a_1 x_1 \sum_{i=1}^n (x_1 - a_i)^{i-1}$$

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_{a_i}$ , and maximum derivative  $\delta_{a_i}$  determined by least-squares analysis.

TK	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$\delta_{a_n}$
	$10^{-6} m^3 \cdot mol^{-1}$						
298.15	1871.5 (8.32)					5.0	9.5

The standard deviations  $\sigma_{a_i}$  of the coefficients  $a_i$  are given in parentheses  $\delta_{a_n} = \max\{12 \frac{\partial v^E}{\partial a_n} \cdot |v^E|, \sigma_{a_n} = 20 \frac{\partial v^E}{\partial a_n} \cdot |v^E|^{1/2} (N - n)^{1/2}\}$   
 $N$ , 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  $0.02$  kg  $m^{-3}$ . The temperature was controlled at  $\pm 0.01$  K with a Beta ultrathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5  $cm^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and n-hexane. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade, degassed ultrasonically, dried over molecular sieves 3A;  $d(0, 298.15 \text{ K}) = 1.1576$ ,  $\rho(298.15 \text{ K}) = 94.89$ ,  $T_g(101.32 \text{ kPa}) = 127.28$   
 2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mole %; degassed ultrasonically, dried over molecular sieves 3A;  $d(0, 298.15 \text{ K}) = 1.3753$ ,  $\rho(298.15 \text{ K}) = 781.66$ , ref. 4,  $T_g(101.32 \text{ kPa}) = 255.39$ .

Errors:  $\delta TK = 0.02$ ,  $\delta a_1 = 0.0025$ ,  $\delta v^E/10^{-6} m^3 \cdot mol^{-1} < 6$ .

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J. Data Ser., Ser. A, Vol. 2003, Pt. 1, 49-57

SELECTED DATA ON MIXTURES  
International Data Series\*

2c. EXCESS VOLUME

National Institute of Standards and Technology, Gaithersburg, MD 20899-1028

Compiled by Thermodynamics Research Center

Components:	1. <i>n</i> -Propanol, C <sub>3</sub> H <sub>8</sub> O [67-63-0] 2. Ethyl ethanoate, C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> [141-78-6]
State:	Binary system, single-phase liquid, pure components, both liquid
Variables:	V <sup>E</sup> , molar excess volume
Parameters:	x <sub>1</sub> , mole fraction of component 1
Parameter:	T, temperature
Constants:	P, pressure
Methods:	Calculation of V <sup>E</sup> from density measurements at constant T and P and variable x <sub>1</sub> ; 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:	Siroz, A.; Macyszko, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

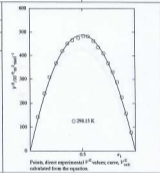
SOURCE OF DATA

Hernández, F.; 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.

TK = 298.15							
x <sub>1</sub>	V <sup>E</sup> /100 m <sup>3</sup> mol <sup>-1</sup>						
0.0145	143						
0.1390	241						
0.1857	309						
0.2580	368						
0.3113	420						
0.3577	452						
0.4055	466						
0.4632	475						
0.5129	484						
0.5554	482						
0.6090	463						
0.6556	436						
0.7026	413						
0.7478	368						
0.7887	330						
0.8350	288						
0.8743	225						
0.9140	158						
0.9619	78						



SMOOTHING EQUATION

$$V_{calc}^E = a_1 x_2 \sum_{i=1}^n (x_1 - x_2)^{i-1}$$

Coefficients a<sub>i</sub> in the smoothing equation, standard deviation σ<sub>a</sub>, and maximum deviation δ<sub>max</sub> determined by least-squares analysis.

TK	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	σ <sub>a</sub>	δ <sub>max</sub>
	10 <sup>-3</sup> m <sup>3</sup> mol <sup>-1</sup>						
298.15	1957.5 (9.46)					7.0	13.1

The standard deviations σ<sub>a</sub> of the coefficients a<sub>i</sub> are given in parentheses. δ<sub>max</sub> = max |V<sup>E</sup><sub>calc</sub> - V<sup>E</sup>|; σ<sub>a</sub> = 200(V<sup>E</sup><sub>calc</sub> - V<sup>E</sup>)<sup>2</sup>/N - x<sub>1</sub><sup>2</sup>/3. N, number of direct experimental values; n, number of coefficients a<sub>i</sub>. All direct experimental values equally weighted.

AUXILIARY INFORMATION

**Apparatus:** The density was determined by an Anton Paar Model DMA-35 vibrating-tube digital densimeter with a precision of ±0.02 kg m<sup>-3</sup>. The temperature was controlled at ±0.01 K with a Heto autothermostat.

**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 toluene. A polynomial equation was used for describing the density-concentration curves.

**Materials:** 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade, degassed ultrasonically, dried over molecular sieves 3A; w(0, 298.15 K) = 1.3752, ρ(298.15 K)/kg m<sup>-3</sup> = 798.77, T<sub>b</sub>(101.32 kPa)/K = 355.39  
2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade, degassed ultrasonically, dried over molecular sieves 3A; w(0, 298.15 K) = 1.3699, ρ(298.15 K)/kg m<sup>-3</sup> = 894.34, T<sub>b</sub>(101.32 kPa)/K = 350.25.

**Error:** ΔTK = 0.02; δa<sub>1</sub> = 0.0005; δσ<sup>2</sup>/10<sup>-6</sup> m<sup>3</sup> mol<sup>-1</sup> < 4.

REFERENCES

1. *Int. J. Ref. Ser. A*, **Goldstein** 38, 1994, 2211.
2. Hernández, F.; Ortega, J. *J. Chem. Eng. Data*, **1997**, *42*, 1090.
3. Ortega, J.; Mason, I. S.; Paz-Andrade, M. I.; Santof, E. *J. Chem. Thermodyn.*, **1985**, *17*, 1127.

80199P-12XSERI-1420

68

Int. J. Ref. Ser., Vol. 34, Chem. Ref. Ser., 1 (2005), 111, 67-72

Compiled by Thermodynamics Research Center

**Component:** 1. 2-Propanol,  $C_3H_8O$  [57-65-7]  
2. Propyl methacrylate,  $C_9H_{10}O_2$  [179-74-7]  
**State:** Binary system, single phase liquid, pure components, both liquid  
**Variables:**  $V^E$ , molar excess volume  
 $x_1$ , mole fraction of component 1  
**Parameters:**  $T$ , temperature  
**Constants:**  $P$ , pressure  
**Method:** Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_1$ , ref. 1

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

SOURCE OF DATA

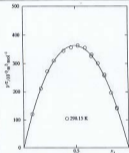
González, C.; Ortega, J.; Hernández, F.; Galván, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes:  $P = 101.32$  kPa.

$T(K) = 298.15$

$x_1$	$V^E(10^3) \text{ m}^3 \text{ mol}^{-1}$				
0.085	121				
0.148	212				
0.231	273				
0.284	318				
0.388	345				
0.469	357				
0.525	363				
0.592	355				
0.651	326				
0.655	331				
0.714	301				
0.775	257				
0.776	261				
0.837	197				
0.890	143				
0.892	141				



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

SMOOTHING EQUATION

$$V^E_{calc} = x_1 x_2 \sum_{j=1}^6 \frac{a_j}{x_1^j} (x_1 - x_2)^{j-1}$$

Coefficients  $a_j$  in the smoothing equation, standard deviation  $\sigma_j$ , and maximum deviation  $\delta_{max}$  determined by least-squares analysis.

TK	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$\delta_{max}$
	$10^3 \text{ m}^3 \text{ mol}^{-1}$						
298.15	3451.4 (7.32)	-37.1 (33.7)	187 (32)			4.6	5.9

The standard deviations  $\sigma_j$  of the coefficients  $a_j$  are given in parentheses  
 $\delta_{max} = \max |V^E_{calc} - V^E|$ ;  $\sigma_j = [20 \sum_{i=1}^N (V^E_i - V^E_{calc})^2]^{-1/2}$   
 $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_j$   
All direct experimental values equally weighted

AUXILIARY INFORMATION

**Apparatus:** The density was determined by an Anton Paar Model DMA-15 vibrating-tube digital densimeter with a precision of  $\pm 0.02 \text{ kg m}^{-3}$ . The temperature was controlled at  $\pm 0.01 \text{ K}$  with a Hele autothermostat.

**Procedure:** The procedure was described in ref. 5. 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 acetone. A polynomial equation was used for describing the density-concentration curve.

**Materials:** 1. Fluka AD (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed azeotropically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $\rho(298.15 \text{ K}) = 1.3752_{10} \text{ kg kg}^{-1}$ ;  $T_b(101.32 \text{ kPa}) = 353.30$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed azeotropically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $\rho(298.15 \text{ K}) = 1.3794_{10} \text{ kg kg}^{-1}$ ;  $T_b(101.32 \text{ kPa}) = 393.75$ .

**Errors:**  $\delta TK = \pm 0.02$ ;  $\delta \rho_1 = 0.000$ ;  $\delta V^E(10^3) \text{ m}^3 \text{ mol}^{-1} < 6$ .

REFERENCES

- Int. Data Ser., Ser. A, Guidelines 7b, 1994, 22(11).
- González, C.; Ortega, J.; Hernández, F.; Galván, S. *J. Chem. Eng. Data*, 1999, 44, 772.
- Ortega, J.; Mitoš, J. S.; Paz-Antón, M. I.; Sandoz, E. *J. Chem. Thermodyn.*, 1985, 17, 1127.

SELECTED DATA ON MIXTURES  
International Data Series\*

2a. EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80505-3328

Compiled by Thermodynamics Research Center

Component: 1. *n*-Propanol, C<sub>3</sub>H<sub>8</sub>O, N7-63-07  
2. Ethyl propanoate, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub>, J187-37-57  
State: Binary system, single-phase liquid, pure components, both liquid  
Variable: V<sup>E</sup>, molar excess volume  
Parameters: x<sub>1</sub>, mole fraction of component 1  
Z, compressibility  
Constant: P, pressure  
Method: Calculation of V<sup>E</sup> from density measurements at constant T and P and variable x<sub>1</sub>, 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: Szwarc, A.; Maczynski, A. Gazeta Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland

SOURCE OF DATA

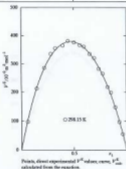
Hernández, F.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: P = 101.32 kPa.

TK = 298.15

x <sub>1</sub>	V <sup>E</sup> (10 <sup>-6</sup> m <sup>3</sup> mol <sup>-1</sup> )						
0.0004	58						
0.0487	215						
0.2191	286						
0.2685	335						
0.3223	355						
0.3945	365						
0.4686	381						
0.5012	378						
0.5575	366						
0.5961	361						
0.6514	335						
0.6923	321						
0.7391	283						
0.7725	266						
0.8092	215						
0.8515	199						
0.8906	148						
0.9291	98						
0.9614	56						



SMOOTHING EQUATION

$$V_{\text{calc}}^E = a_1 a_2 \sum_{i=1}^5 (x_1 - a_3)^{2i-1}$$

Coefficients a<sub>i</sub> in the smoothing equation, standard deviation σ<sub>a</sub>, and maximum deviation δ<sub>m</sub> determined by least-squares analysis.

TK	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	δ <sub>m</sub>
	10 <sup>-6</sup> m <sup>3</sup> mol <sup>-1</sup>						
298.15	1513.5 (8.1)	-159.4 (36.3)	207 (0)			4.9	8.2

The standard deviations (σ<sub>a</sub>) of the coefficients a<sub>i</sub> are given in parentheses  
δ<sub>m</sub> = max{|V<sup>E</sup><sub>calc</sub> - V<sup>E</sup>|}; σ<sub>a</sub> = [(10<sup>6</sup> V<sup>E</sup> - V<sup>E</sup>)<sup>2</sup> / (N - 6)]<sup>0.5</sup>  
N, number of direct experimental values; n, number of coefficients a<sub>i</sub>  
All direct experimental values equally weighted

AUXILIARY INFORMATION

Apparatus: The density was determined by an Anton Paar Model D50A-55 vibrating-tube digital densimeter with a precision of ±0.02 kg m<sup>-3</sup>. The temperature was controlled at ±0.01 K with a Hele ultrathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in homometrically sealed 2.5 cm<sup>3</sup> glass vials. The apparatus was calibrated with doubly distilled and degassed water and anisole. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; ρ(298.15 K) = 1.3732, ρ(298.15 K) kg m<sup>-3</sup> = 780.71, T<sub>b</sub>(101.32 kPa)/K = 355.38.  
2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A; ρ(298.15 K) = 1.3811, ρ(298.15 K) kg m<sup>-3</sup> = 883.93, T<sub>b</sub>(101.32 kPa)/K = 371.92.

Errors: ΔTK = 0.02, δx<sub>1</sub> = 0.0003, δV<sup>E</sup> (10<sup>-6</sup> m<sup>3</sup> mol<sup>-1</sup>) < 6.

REFERENCES

- Int. Data Ser., Ser. A, Guidelines, 1994, 22(1).
- Hernández, F.; Ortega, J. *J. Chem. Eng. Data*, 1997, 42, 1090.
- Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Jiménez, E. *J. Chem. Thermodyn.*, 1985, 17, 1127.

Received: January 1, 2003

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

Published: January 31, 2003

SELECTED DATA ON MIXTURES  
International Data Series\*

No. EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80505-3338

Compiled by Thermodynamics Research Center

Components: 1. 2-Propanol,  $C_3H_8O$  (67-63-2)  
2. Propyl ethanoate,  $C_5H_{10}O_2$  (100-60-4)

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

Variables:  $V^E$ , molar excess volume  
 $x_1$ , mole fraction of component 1

Parameters:  $T$ , temperature  
Constants:  $P$ , pressure

Method: Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_1$ , ref. 1

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)

Editor(s) Skrzec, A.; Mącznycki, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

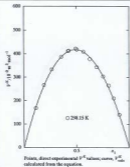
González, C.; Ortega, J.; Hernández, F.; Galván, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes:  $P = 101.32$  kPa.

UK = 298.15

$x_1$	$V^E/10^{-6}$ $m^3 mol^{-1}$					
0.012	168					
0.039	267					
0.264	534					
0.354	385					
0.428	432					
0.427	434					
0.494	432					
0.503	435					
0.556	409					
0.627	378					
0.692	344					
0.752	364					
0.803	265					
0.852	219					
0.903	141					



SMOOTHING EQUATION

$$V^E_{calc} = x_1 x_2 \sum_{j=1}^6 (V_j - x_j)^{j-1}$$

Coefficients  $a_j$  in the smoothing equation, standard deviation  $\sigma_{jk}$ , and maximum deviation  $\delta_{jk}$  determined by least-squares analysis.

UK	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$\delta_{jk}$
	$V^E/10^{-6}$ $m^3 mol^{-1}$						
298.15	1674.7 (6.25)	-73.1 (17.8)				4.8	9.3

The standard deviations ( $\sigma_j$ ) of the coefficients  $a_j$  are given in parentheses.  $\delta_{jk} = \max |V^E_{calc} - V^E|$ ;  $\sigma_{jk} = [2(V^E_{calc} - V^E)^2 / (N - n)]^{1/2}$ .  $N$ , number of direct experimental values;  $n$ , number of coefficients  $a_j$ . 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  $\pm 0.02$  kg m<sup>-3</sup>. The temperature was controlled at  $\pm 0.01$  K with a flow thermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 25 cm<sup>3</sup> glass vials. The apparatus was calibrated with doubly distilled and degassed water and ethanol. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed azeotropically, dried in darkness over molecular sieves  $3A$ ; no significant impurities by glc;  $n_D^{20}$  298.15 K = 1.3732,  $\rho$ (298.15 K) kg m<sup>-3</sup> = 781.33,  $T_c$ (101.32 kPa)/K = 353.36.  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed azeotropically, dried in darkness over molecular sieves  $3A$ ; no significant impurities by glc;  $n_D^{20}$  298.15 K = 1.3816,  $\rho$ (298.15 K) kg m<sup>-3</sup> = 882.67,  $T_c$ (101.32 kPa)/K = 374.31.

Errors:  $\Delta T_K = 0.02$ ;  $\Delta x_1 = 0.001$ ;  $\Delta V^E/10^{-6}$  m<sup>3</sup> mol<sup>-1</sup>  $\leq 5$ .

REFERENCES

- Int. Data Ser., Ser. A, Goldfarb JB, 1994, 22(1).
- González, C.; Ortega, J.; Hernández, F.; Galván, S. *J. Chem. Eng. Data*, 1999, 44, 772.
- Ortega, J.; Mateo, J. S.; Pao-Andrade, M. J.; Jiménez, E. *J. Chem. Thermodyn.*, 1998, 17, 1127.

JPL-1000-1-EXCESS-VOLUME

69

An IUPAC Pure Substances Data Series, Vol. 1, 1992, 1-11, 69-73

SELECTED DATA ON MIXTURES  
International Data Series\*

2c. EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80505-3328

NIST REFERENCE DATA

Components: 1. 2-Propanol,  $C_3H_8O$  (67-63-6)  
2. Ethyl butanoate,  $C_6H_{12}O_2$  (111-54-4)

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

Variables:  $V^E$ , molar excess volume  
 $x_1$ , mole fraction of component 1

Parameters:  $T$ , temperature  
 $P$ , pressure

Method: Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_1$ , ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Filoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 36071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

SOURCE OF DATA

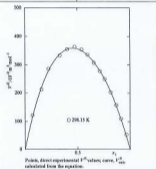
Hernández, F.; Ortega, J. (Laboratorio de Termodinámica y Filoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes:  $P = 101.32$  kPa

$TK = 298.15$

$x_1$	$V^E/10^{-6}$ $m^3 mol^{-1}$				
0.0714	122				
0.1365	235				
0.2253	286				
0.3324	335				
0.4027	355				
0.4743	363				
0.5407	354				
0.5967	336				
0.6565	308				
0.7139	278				
0.7585	258				
0.8147	203				
0.8694	158				
0.9143	118				
0.9644	54				



SMOOTHING EQUATION

$$V_{min}^E = v_0 + v_1 \sum_{i=1}^6 (x_i - x_j)^{i+1}$$

Coefficients  $v_i$  in the smoothing equation, standard deviation  $\sigma_{v_i}$ , and maximum deviation  $\delta_{v_i}$  determined by least-squares analysis.

TK	$v_0$	$v_1$	$v_2$	$v_3$	$v_4$	$v_5$	$v_6$
	$m^3 mol^{-1}$						
298.15	1438.1 (8.2)	-238.1 (6.8)	195 (7)			4.5	7.5

The standard deviation  $\sigma_{v_i}$  of the coefficients  $v_i$  are given in parentheses  $\delta_{v_i} = \max |V_{calc}^E - V^E|$ ;  $\sigma_{v_i} = (20 \sum_{j=1}^N (V_{calc}^E - V^E)^2 / (N - 6))^{1/2}$ ;  $N$ , number of direct experimental values;  $n$ , number of coefficients;  $v_j$ . All direct experimental values equally weighted.

AUXILIARY INFORMATION

Apparatus: The density was determined by an Anton Paar Model DMA-15 vibrating-tube digital densimeter with a precision of  $\pm 0.02$  kg  $m^{-3}$ . The temperature was controlled at  $\pm 0.01$  K with a Hele-attenuation.

Procedure: The procedure was described in ref. 1. Mixtures were prepared by weighing in hermetically sealed 2.5  $cm^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and benzene. A polynomial equation was used for describing the density-concentration curve.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A,  $n(0, 298.15$  K) = 1.3712,  $\rho(298.15$  K)  $kg m^{-3}$  = 788.77,  $T_b(101.32$  kPa)  $K$  = 353.50.  
2. Fluka AG (Buchs, St. Gallen, Switzerland), highest commercial grade; degassed ultrasonically, dried over molecular sieves 3A,  $n(0, 298.15$  K) = 1.3894,  $\rho(298.15$  K)  $kg m^{-3}$  = 873.94,  $T_b(101.32$  kPa)  $K$  = 394.18.

Errors:  $\delta TK = 0.02$ ,  $\delta v_1 = 0.0005$ ,  $\delta V^E/10^{-6} m^3 mol^{-1} < 6$ .

REFERENCES

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- Hernández, F.; Ortega, J. *J. Chem. Eng. Data*, 1997, 42, 1899.
- Ortega, J.; Mateo, J. S.; Paz-Andrade, M. I.; Jiménez, E. *J. Chem. Thermodyn.*, 1988, 20, 1127.

Received: January 1, 2005

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SELECTED DATA ON MIXTURES  
International Data Series\*

In EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80505-3338

Compiled by Thermodynamics Research Center

**Components:** 1. 2-Propanol,  $C_3H_8O$  [157-05-0]  
2. Propyl propanoate,  $C_6H_{12}O_2$  [106-36-5]  
**State:** Binary system, single-phase liquid; pure components, both liquid  
**Variables:**  $V^E$ : molar excess volume  
 $x_1$ : molar fraction of component 1  
**Parameters:**  $T$ : temperature  
**Constants:**  $P_1$ : pressure  
**Method:** Calculation of  $V^E$  from density measurements at constant  $T$  and  $P$  and variable  $x_1$ ; ref. 1

**Author(s):** Ortega, J., Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35017 Las Palmas de Gran Canaria, Canary Islands, Spain

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

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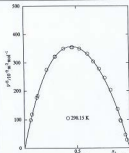
González, C.; Ortega, J.; Hernández, P.; Ordoño, S., Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain; ref. 2

DIRECT EXPERIMENTAL VALUES

Notes:  $P = 101.32$  kPa.

$T/K = 298.15$

$x_1$	$V^E/10^{-6}$ $m^3 \cdot mol^{-1}$	$x_1$	$V^E/10^{-6}$ $m^3 \cdot mol^{-1}$
0.060	96	0.858	47
0.072	115	0.872	29
0.120	177		
0.128	185		
0.217	275		
0.298	321		
0.298	322		
0.379	349		
0.437	334		
0.465	334		
0.531	349		
0.606	391		
0.662	394		
0.715	278		
0.767	266		
0.823	269		
0.888	137		
0.913	98		
0.917	95		



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

SMOOTHING EQUATION

$$V^E_{\text{calc}} = x_1 x_2 \sum_{i=1}^6 (x_i - x_j)^{i-1}$$

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_{a_i}$  and maximum deviation  $R_{\text{max}}$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$R_{\text{max}}$
	$10^{-6} m^3 \cdot mol^{-1}$						
298.15	3430.0 (8.0)	-222.8 (15.3)	133 (25)			6.8	8.6

The standard deviations  $\sigma_{a_i}$  of the coefficients  $a_i$  are given in parentheses.  
 $a_0 = \max[V^E_{\text{calc}} - V^E]$ ;  $a_4 = [2(1 - x_1) - V^E] / (1 - x_1)^{1/2}$   
 $N$ : 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-35 vibrating-tube digital densimeter with a precision of  $\pm 0.02$  kg m $^{-3}$ . The temperature was controlled at  $\pm 0.01$  K with a flow thermostat.

**Procedure:** The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm $^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and benzene. A polynomial equation was used for describing the density-concentration curve.

**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;  $\rho(0, 298.15 \text{ K}) = 1.3752$ ,  $\rho(298.15 \text{ K}) \text{ kg m}^{-3} = 781.53$ ,  $T_f(101.32 \text{ kPa}) = 355.36$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A; no significant impurities by glc;  $\rho(0, 298.15 \text{ K}) = 1.3806$ ,  $\rho(298.15 \text{ K}) \text{ kg m}^{-3} = 875.61$ ,  $T_f(101.32 \text{ kPa}) = 395.58$ .

**Errors:**  $\pm 7$  K = 0.02;  $\Delta x_1 = 0.001$ ;  $\Delta V^E/10^{-6} m^3 \cdot mol^{-1} < 6$ .

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

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**Compos:** 1. 2-Propanol,  $C_3H_8O$  [67-63-0]  
2. Propyl acetate,  $C_5H_{10}O_2$  [103-66-8]  
**State:** Binary system, single-phase liquid, pure components, both liquid  
**Variable:**  $V^E$ , molar excess volume  
**Parameters:**  $x_1$ , molar fraction of component 1  
**Constants:**  $T$ , temperature  
**Method:** Calculation of  $V^E$  from density measurements at constant  $T$  and P and variable  $x_1$ , ref. 1

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**Editor(s):** Sliemers, A.; Maczynski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

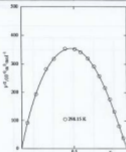
González, C.; Ortega, J.; Hernández, P.; Galván, S. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingeniería Industrial, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), ref. 2

DIRECT EXPERIMENTAL VALUES

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

$T/K = 298.15$

$x_1$	$V^E/10^{-6} \text{ m}^3 \text{ mol}^{-1}$				
0.055	92				
0.137	294				
0.234	282				
0.309	318				
0.416	353				
0.507	352				
0.563	341				
0.632	319				
0.699	291				
0.739	258				
0.795	216				
0.839	176				
0.880	132				
0.928	81				
0.964	39				



Points, direct experimental  $V^E$  values; curve,  $V^E$  calculated from the equation.

SMOOTHING EQUATION

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

Coefficients  $a_i$  in the smoothing equation, standard deviation  $\sigma_{ij}$ , and maximum deviation  $\delta_{\text{max}}$  determined by least-squares analysis.

T/K	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$\sigma_4$	$\delta_{\text{max}}$
	$\text{m}^3 \text{ mol}^{-1}$						
298.15	1034.0 (4.7)	-158.7 (7.5)	89 (20)	-228 (43)		2.4	4.0

The standard deviations  $\sigma_{ij}$  of the coefficients  $a_i$  are given in parentheses.  $\delta_{\text{max}} = \max |V_{\text{calc}}^E - V^E|$ ;  $\sigma_{ij} = [20(V_{\text{calc}}^E - V^E)^2 / (N - i)]^{1/2}$ .  $N$ , number of direct experimental values;  $i$ , 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  $\pm 0.02 \text{ kg m}^{-3}$ . 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 25  $\text{cm}^3$  glass vials. The apparatus was calibrated with doubly distilled and degassed water and toluene. A polynomial equation was used for describing the density-concentration curve.

**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;  $\rho(0, 298.15 \text{ K}) = 1.1752$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 381.38$ ,  $T_f(101.32 \text{ kPa})/\text{K} = 315.38$ .  
2. Aldrich (Steinheim, Germany), highest commercial grade; degassed ultrasonically, dried in darkness over molecular sieves 3A, no significant impurities by glc;  $\rho(0, 298.15 \text{ K}) = 1.3075$ ,  $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 668.01$ ,  $T_f(101.32 \text{ kPa})/\text{K} = 416.57$ .

**Errors:**  $\delta T/K = 0.02$ ,  $\delta \rho_1 = 0.006$ ,  $\delta V^E/10^{-6} \text{ m}^3 \text{ mol}^{-1} < 3$ .

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