

SELECTED DATA ON MIXTURES
International Data Series*

2b. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamic Research Center

Components: 1. Ethyl acetate, $C_4H_8O_2$ (141-38-6)
2. 1-Chloropropane, C_3H_7Cl (543-59-6)
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 Filoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35017 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

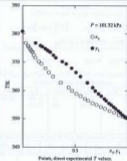
SOURCE OF DATA

Ortega, J.; Peña, J. A. 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

$P/101.32$

x_2	TK	y_1	x_1	TK	y_1
0.0008	348.90	0.0000	0.5534	338.25	0.7907
0.8239	326.85	0.1249	0.5938	337.25	0.7800
0.8505	325.90	0.1714	0.6263	336.65	0.7963
0.8736	325.55	0.1891	0.6674	335.75	0.8235
0.8790	324.80	0.2375	0.7834	335.15	0.8451
0.8797	324.35	0.2357	0.7434	334.35	0.8679
0.8867	323.95	0.2505	0.7843	333.75	0.8878
0.8963	323.65	0.2631	0.8292	332.95	0.9118
0.1084	322.55	0.2844	0.8726	332.25	0.9329
0.1234	321.65	0.3068	0.9067	331.45	0.9544
0.1546	320.25	0.3792	0.9538	330.65	0.9737
0.1792	319.45	0.4158	0.9787	330.55	0.9868
0.2175	317.85	0.4683	1.0000	330.30	1.0000
0.2497	316.35	0.5087			
0.2897	314.95	0.5526			
0.3634	313.85	0.6091			
0.4388	313.15	0.6897			
0.4728	312.05	0.6949			
0.5143	310.05	0.7253			



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebullometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 30 cm³, 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 a Fisher model VKI1100 pressure controller. The pressure was measured by a MGS Instrument Systems with reading intervals 1 Pa; accuracy of the reading > 20 Pa. The temperatures were measured by a digital thermometer Comark Electronics model 6800 using a PT-100 sensor with reading intervals 50 mK.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their density at 298.15 K with an Anton Paar model 4605D vibrating-tube densimeter calibrated with water and acetone, ref. 4. A fourth-order polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty was ± 0.0025 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.5 mass %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.3706$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 894.34$.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.4899$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 876.92$.

Notes: 1) $P/\text{Pa} = 0.1$; 2) $P/\text{Pa} = 200$; 3) $\Delta T_{\text{b}} = 0.085$; 4) $\Delta T_{\text{b}} = 0.1$.

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1. *Int J Refract Prop*, **10**, 4, *Optical Prop*, 1994, 226-3.
2. Ortega, J.; Peña, J. A. *J. Chem. Eng. Data*, **1994**, *27*, 351.
3. Ortega, J.; Peña, J. A.; de Alencastro, C. *J. Chem. Eng. Data*, **1996**, *31*, 339.
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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 Thermodynamic Research Center

Components:	1. Ethyl ethanoate, $C_4H_8O_2$ [141-28-4] 2. 1-Chloroethane, C_2H_5Cl [741-50-6]
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:	Calculation from direct experimental liquid-vapor equilibrium temperature, T_{exp} data at variable x_1 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)
Editor(s): Oraz, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

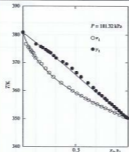
SOURCE OF DATA

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

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

		P/P ₁ = 101.32					
x_1	T/K	y_1					
0.00	380.91	0.0000					
0.05	376.40	0.1587					
0.10	373.03	0.2713					
0.15	370.36	0.3932					
0.20	368.16	0.4266					
0.25	366.29	0.4650					
0.30	364.63	0.5302					
0.40	361.84	0.6208					
0.50	359.45	0.6997					
0.60	357.32	0.7679					
0.70	355.38	0.8318					
0.75	354.46	0.8643					
0.80	353.58	0.8903					
0.85	352.72	0.9188					
0.90	351.89	0.9463					
0.95	351.08	0.9736					
1.00	350.30	1.0000					

Standard deviation $\sigma(T)$, relative standard deviation 100 $\sigma(T)/T$, and absolute maximum deviation $\Delta_{max}(T)/K$ at P/P₁ = 101.32 are: exp.: 0.799, 0.887, 1.192.



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

EQUATIONS

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

$$v_1 = \exp\left[-(a_1 + \frac{a_2^2}{4T})\right] \quad v_2 = \exp\left[-(a_2 + \frac{a_1^2}{4T})\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 v_i P_i^s \exp\left[\frac{P_i^s - (P_i^s - P_i^s T^s - T^s) - 2P_i^s(1 - x_1)^2}{RT}\right]$$

$$\rho_1^s = G^E - x_2(G^E / \Delta v_1)_{exp} \quad \rho_2^s = G^E - x_1(G^E / \Delta v_2)_{exp}$$

$$B_{12}^E = B_{12} - (B_{11} + B_{22})/2; \quad P_i^s/P_1^s = \exp[A_i + B_i/(C_i + TX)]$$

COEFFICIENTS IN THE EQUATIONS

P/P ₁	a_1/K	a_2/K^2	a_3/K	a_4/K^2
101.32	-189.82 (13.2)	0 00	323.48 (27.4)	0 00

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

P/P ₁	A_1	B_1	C_1	A_2	B_2	C_2
101.32	14.30449	-3153.18	-37.47	13.48479	-2026.95	-38.15

AUXILIARY INFORMATION

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

Computations: The 22 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 .

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_{pp} , ref. 5, and the molar volume under saturation pressure $V_{1,T}^s$, ref. 6.

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

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- Wilson, G. M. *J. Am. Chem. Soc.*, 1964, 86, 127.
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- Yeo, L. C.; Woods, S. S. *AIChE J.*, 1966, 12, 93.

SELECTED DATA ON MIXTURES

International Data Series*

36. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamic Research Center

Components: 1. Ethyl ethanoate, $C_4H_8O_2$ (747-79-6)
2. 1-Chloroethane, C_2H_5Cl (544-18-5)

State: Binary azeotropic, 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

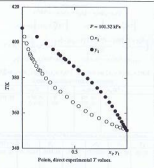
Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35011 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

SOURCE OF DATA
Ortega, J.; Peña, J. A. (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

$P/P_0 = 101.32$					
x_1	TK	y_1	x_2	TK	y_2
0.0000	485.85	0.0000	0.5308	364.05	0.0003
0.0221	483.85	0.1409	0.6061	361.30	0.0086
0.0418	399.35	0.2208	0.6647	358.25	0.0121
0.0539	386.15	0.2993	0.7336	357.35	0.0323
0.0739	383.65	0.3493	0.8054	355.35	0.0515
0.0885	382.75	0.3657	0.8601	353.85	0.0646
0.0990	381.85	0.4036	0.9043	352.65	0.0782
0.1026	380.45	0.4147	0.9369	351.95	0.0824
0.1180	388.85	0.4494	0.9666	351.45	0.0824
0.1338	386.75	0.4927	1.0000	350.30	1.0000
0.1514	384.65	0.5356			
0.1767	384.25	0.5437			
0.1989	382.35	0.5883			
0.2217	379.85	0.6299			
0.2685	377.55	0.6675			
0.3149	374.55	0.7167			
0.3658	372.35	0.7325			
0.4282	369.35	0.7929			
0.4833	366.35	0.8330			



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass stillometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm³; ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The stillometer was connected to a vacuum pump and a Fisher model VKS100 pressure controller. The pressure was measured by a MKS Instrument System with reading intervals 1 Pa; accuracy of the reading > 20 Pa. The temperatures were measured by a digital thermometer Comark Electronics model 6808 using a PT-100 sensor with reading intervals 50 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 4090D vibrating tube densimeter calibrated with water and toluene; ref. 4. A fourth-order polynomial equation describing the density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty was ± 0.0025 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.3 mass %; degassed ultrasonically; dried over molecular sieves 3A; ρ_{20}^L , 288.15 K = 1.3701, $\rho_{298.15}^L$ K298 = 894.34.
2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically; dried over molecular sieves 3A; ρ_{20}^L , 298.15 K = 1.4174, $\rho_{298.15}^L$ K298 = 875.35.

Notes: 1) $T/K = 0.1$; 2) $P/P_0 = 298$; 3) $\Delta_{\text{ref}} = 0.003$; 4) $\Delta_{\text{ref}} = 0.06$.

REFERENCES
1. Int. DATA Ser., Ser. A, *Guilford*, 1994, 23(4).
2. Ortega, J.; Peña, J. A. *J. Chem. Eng. Data*, 1994, 27, 331.
3. Ortega, J.; Peña, J. A.; de Alencar, C. *J. Chem. Eng. Data*, 1986, 31, 338.
4. Ortega, J.; Mateo, J. S.; Paz-Audaz, M. I.; Ramos, E. *J. Chem. Thermodyn.*, 1995, 17, 1123.

SELECTED DATA ON MIXTURES

International DATA Series*

3a. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamic Research Center

Components:	1. Ethyl ethanoate, $C_4H_8O_2$ (141-26-0) 2. 1-Chloroethane, C_2H_5Cl (78-07-5)
State:	Binary system, single-phase liquid in equilibrium with vapor; pure components, both liquid in equilibrium with vapor
Variables:	T , temperature x_i , mole fraction of component i in liquid phase y_i , mole fraction of component i in vapor phase
Parameters:	P , pressure
Method:	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 Psicocapilares, Escuela Superior de Ingenieros Industriales, de Icaña 26, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain)

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

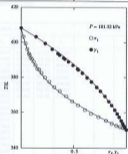
SOURCE OF DATA

Ortega, J.; Peña, E. A. (Laboratorio de Termodinámica y Psicocapilares, 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	TK	y_1			
0.00	408.05	0.0000			
0.05	397.62	0.2799			
0.10	390.64	0.4368			
0.15	385.52	0.5382			
0.20	381.49	0.6008			
0.25	378.14	0.6668			
0.30	375.28	0.7122			
0.40	370.29	0.7834			
0.50	366.08	0.8385			
0.60	362.35	0.8839			
0.70	358.96	0.9204			
0.75	357.37	0.9563			
0.80	355.85	0.9512			
0.85	354.38	0.9649			
0.90	352.97	0.9776			
0.95	351.61	0.9892			
1.00	350.30	1.0000			

Standard deviation $\sigma(T)$, TK, relative standard deviation $100\sigma(T)/T$, and absolute maximum deviation $\Delta_{max}(T)/TK$ at PMPs = 101.32 are resp.: 0.978, 1.102, 0.762.



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

EQUATIONS

$$G^E RT = -x_1 \ln v_1 + x_2 \ln v_2 - x_1 x_2 (x_1 + x_2)$$

$$v_1 = \exp \left[-\ln v_1 + \frac{G^E}{RT} \right] \quad v_2 = \exp \left[-\ln v_2 + \frac{G^E}{RT} \right]$$

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

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

$$R_{i,1}^L = R_{i,2}^L - (R_{i,1}^L + R_{i,2}^L) (2 - y_i) - P_i^s / P; \quad P_i^s / P = \exp [A_i + B_i / (C_i + 20K)]$$

COEFFICIENTS IN THE EQUATIONS

PMPs	a_i/K	a_{ij}/K^2	a_{ij}/K	a_{ij}/K^2
101.32	-150.36 (12.8)	0 (0)	425.44 (27.2)	0 (0)

The standard deviations $\sigma(a_{ij})$ of the coefficients a_{ij} are given in parentheses.

PMPs	A_i	B_i	C_i	A_i	B_i	C_i
101.32	14.76403	-3035.18	-37.67	15.92293	-3189.26	-45.29

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 .

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_{ij} , ref. 5, and the molar volumes under saturation pressure V_i^L , ref. 6.

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

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1. *Int. DATA Ser., Ser. A, Collected Vol.*, 1995, 2(2).
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5. Thompson, C. *AIChE J.*, 1974, 20, 383; 1975, 21, 827.
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