

Compiled by Thermodynamics Research Center

Component:	1. Methyl ethanoate, $C_3H_6O_2$ (79-20-6) 2. 1-Chloropentane, $C_5H_{11}Cl$ (1163-59-9)
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): 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)

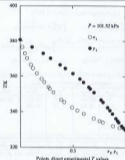
Edited by: Sierwa, A.; Maryczka, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

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

$P/P_1 = 101.32$					
x_1	TK	y_1	x_1	TK	y_1
0.0000	346.91	0.0000	0.7854	334.15	0.9388
0.0207	376.65	0.1131	0.8835	332.15	0.9659
0.0447	373.10	0.2195	0.9404	331.13	0.9885
0.0649	370.35	0.2891	1.0000	330.05	1.0000
0.1011	366.70	0.3832			
0.1288	364.76	0.4291			
0.1579	361.75	0.5009			
0.2026	358.65	0.5887			
0.2283	356.75	0.6034			
0.2673	354.80	0.6332			
0.2885	353.80	0.6682			
0.3156	351.85	0.7036			
0.3891	348.95	0.7791			
0.4183	348.65	0.7899			
0.4917	342.65	0.8349			
0.5424	340.95	0.8336			
0.6032	339.05	0.8784			
0.7081	336.35	0.9102			
0.7350	335.85	0.9254			



AUXILIARY INFORMATION

Apparatus:	The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a charge capacity of 50 cm ³ , ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and a Fisher model VQH100 pressure controller. The pressure was measured by a MEX Indastrom System 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 densities at 286.15 K with an Anton Paar model 60602 vibrating-tube densimeter calibrated with water and toluene, ref. 4. A fourth-order polynomial equation describing density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty ± 0.0025 mole fraction.
Materials:	1. Fika AG (Buchs, St. Gallen, Switzerland), purity > 99.95 mass %, degassed ultrasonically, dried over molecular sieves 3A; $\rho(286.15 \text{ K}) = 1.3190$; $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 927.03$. 2. Fika AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(286.15 \text{ K}) = 1.4090$; $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 876.92$.
Error:	$\pm 0.7 \text{ K}$; $\pm 4 \text{ Pa}$; $ u_{x_1} = 0.003$; $ u_{y_1} = 0.01$.

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1. *Int J Ref Data Ser, Ser A*, Guilleme M, 1994, 23(4).
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3. Ortega, J.; Peña, J. A.; de Abajo, C. *J. Chem. Eng. Data*, 1986, 31, 339.
4. Ortega, J.; Mateo, F. S.; Paz-Aredero, M. L.; Sanchez, E. *J. Chem. Thermodyn.*, 1985, 17, 1127.

SELECTED DATA ON MIXTURES

International Data Series*

3rd LIQUID-VAPOR EQUILIBRIUM

Compiled by Thermodynamics Research Center

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

Components: 1. Methyl ethanoate, $C_2H_5CO_2$ [79-20-9]
2. 1-Chloroethane, C_2H_5Cl [78-10-5]

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: 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, de calle No. Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

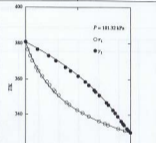
Editor(s): Onor, P. (Wydział Chemii, Uniwersytetu Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

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_i .

101.32			181.32		
x_1	T/K	y_1	x_1	T/K	y_1
0.80	380.94	0.0000	0.80	380.94	0.0000
0.85	373.46	0.2268	0.85	373.46	0.2268
0.10	367.41	0.3851	0.10	367.41	0.3851
0.15	362.40	0.4998	0.15	362.40	0.4998
0.20	358.20	0.5877	0.20	358.20	0.5877
0.25	354.62	0.6521	0.25	354.62	0.6521
0.30	351.58	0.7047	0.30	351.58	0.7047
0.40	346.47	0.7826	0.40	346.47	0.7826
0.50	342.49	0.8374	0.50	342.49	0.8374
0.60	339.26	0.8790	0.60	339.26	0.8790
0.70	336.56	0.9127	0.70	336.56	0.9127
0.75	335.35	0.9238	0.75	335.35	0.9238
0.80	334.22	0.9421	0.80	334.22	0.9421
0.85	333.13	0.9561	0.85	333.13	0.9561
0.90	332.09	0.9701	0.90	332.09	0.9701
0.95	331.07	0.9846	0.95	331.07	0.9846
1.00	330.05	1.0000	1.00	330.05	1.0000



EQUATIONS

$$G^E RT = -x_1 \ln \gamma_1 + x_2 \ln \gamma_2 - x_1 x_2 (x_1 + x_2) \tau$$

$$\tau_1 = \exp \left[-A_1 + \frac{B_1}{T} \right] \quad \tau_2 = \exp \left[-A_2 + \frac{B_2}{T} \right]$$

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

$$\rho_i^s = G^E - x_i (HG^E / \Delta h_i)_{2,2} \quad \rho_2^s = G^E - x_1 (HG^E / \Delta h_1)_{2,2}$$

$B_{12}^E - B_{22}^E - (B_{11}^E + B_{22}^E) x_1^2 = P_1^s / P_2^s$; $P_i^s / P^s = \exp [A_i + B_i / (C_i + T)]$

COEFFICIENTS IN THE EQUATIONS

P/kPa	A_i /K	B_i /K ²	C_i /K	τ_{ij} /K ²
101.32	250.84	-67.506	0	0
181.32	163.4	0	18.4	0

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

P/kPa	A_1	B_1	C_1	A_2	B_2	C_2
101.32	14.24546	-2662.78	-53.46	13.68679	-2936.55	-58.15

Standard deviation $\sigma(T)$, relative standard deviation $\sigma(T)/T$, and absolute maximum deviation $\Delta_{max}(T)/K$ at $P/kPa = 101.32$ are resp. 0.588, 1.548, 1.971.

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

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

Computations: The 25 T_{exp} data at 181.32 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 impurities 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 $\sigma(T) = [217 \cdot T_{exp}^{-2} / (N - 2)]^{1/2}$, Relative standard deviation $100\sigma(T)/T = 100[217 \cdot T_{exp}^{-2} / (N - 2)]^{1/2}$, N , number of experimental points, ref. 2, n , number of coefficients in the smoothing equation.

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Int. Data Ser., Ser. A, Thermodynamic Properties of Non-reacting Binary Systems, Vol. 30, No. 1, 2003, pp. 73-76

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. Methyl ethanoate, $C_3H_6O_2$ (79-20-9)
2. 1,4-Dioxane, $C_4H_8O_2$ (744-70-3)

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

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

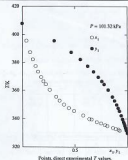
Edited by: Szwarc, A.; Moczyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Replanta 40/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

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

DIRECT EXPERIMENTAL VALUES

$P/kPa = 101.32$						
x_1	T/K	y_1	x_2	T/K	y_2	
0.0000	406.05	0.0000	0.7447	336.90	0.8699	
0.0407	395.65	0.3667	0.7873	335.76	0.9148	
0.0754	387.48	0.4677	0.8099	333.15	0.9771	
0.1045	382.38	0.5547	0.8263	333.75	0.9832	
0.1272	377.68	0.6234	0.8487	333.68	0.9863	
0.1504	373.58	0.6867	0.9147	332.68	0.9876	
0.1794	369.78	0.7285	0.9254	331.95	0.9905	
0.2022	366.78	0.7579	1.0000	330.05	1.0000	
0.2303	364.58	0.7902				
0.2613	368.68	0.8185				
0.3224	355.85	0.8290				
0.3551	353.05	0.8389				
0.3971	358.28	0.8978				
0.4427	367.85	0.9128				
0.4925	343.88	0.9284				
0.5793	342.55	0.9421				
0.6390	348.00	0.9545				
0.6587	338.70	0.9561				
0.7088	337.83	0.9650				



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 50 cm³, ref. 1. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and a Fisher model VQ1100 pressure controller. The pressure was measured by a MKS Instruments System with reading intervals 1 Pa; accuracy of the reading > 20 Pa. The temperatures were measured by a digital thermometer Conach Electronics model 6800 using a PT-100 sensor with reading intervals 0.01 K.

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 60902 vibrating-tube densimeter calibrated with water and benzene, ref. 4. A fourth order polynomial equation describing density-concentration curve obtained from mixtures of known composition was used in the calculations. Estimated uncertainty ± 0.0025 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99.99 mass %, degassed ultrasonically, dried over molecular sieves 5A; $\rho(298.15 \text{ K}) = 1.3390$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 927.02$.

2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mass %, degassed ultrasonically, dried over molecular sieves 5A; $\rho(298.15 \text{ K}) = 1.4174$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.33$.

Purity: $[x_1] = 0.4$; $[x_2] = 200$; $[y_1] = 0.003$; $[y_2] = 0.01$.

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3. Ortega, J.; Peña, J. A.; de Alencar, C. *J. Chem. Eng. Data*, 1986, 31, 339.
4. Ortega, J.; Matos, J. S.; Paz-Andrade, M. I.; Amaro, B. *J. Chem. Thermodyn.*, 1988, 17, 1127.

SELECTED DATA ON MIXTURES

International Data Series*

3a. LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

Components: 1. Methyl ethanoate, C₃H₆O₂ (79-20-9)
2. 1-Cloroetano, C₂H₅Cl (74-47-5)

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: Calculation from direct experimental liquid-vapor equilibrium temperatures, T_{exp} data at variable x₁ and constant P; ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, of table No. Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

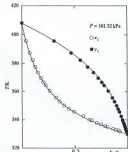
Edited by: Cray, P. (Wydział Chemii, Uniwersytet Warszawski, ul. Pasteura 1, 02-093 Warszawa, Poland)

SOURCE OF DATA

Ortega, J.; Peto, 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

Note: The table reports smoothed values of T and calculated values of y₁

P/MPa = 101.32		
x ₁	T/K	y ₁
0.00	406.09	0.0000
0.05	393.28	0.3661
0.10	382.16	0.5074
0.15	373.74	0.6068
0.20	367.13	0.7028
0.25	361.80	0.8143
0.30	357.41	0.8588
0.40	356.58	0.8987
0.50	345.46	0.9284
0.60	341.44	0.9488
0.70	338.33	0.9642
0.75	336.66	0.9767
0.80	335.27	0.9766
0.85	333.85	0.9826
0.90	332.64	0.9883
0.95	331.35	0.9940
1.00	330.65	1.0000



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

EQUATIONS

$$G^E RT = -x_1 B_1(x_1 + x_2) - x_2 B_2(x_2 + x_1)$$

$$v_1 = \exp\left[-A_1 + \frac{B_1}{T}\right] \quad v_2 = \exp\left[-A_2 + \frac{B_2}{T}\right]$$

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

$$P_1^s = G^E - x_1 B_1^E(x_1 + x_2) \quad P_2^s = G^E - x_2 B_2^E(x_1 + x_2)$$

$$B_{12}^E = B_{12}^E - G_{12}^E - G_{11}^E + B_{11}^E/2; y_1 = P/P; P_i^s/MPa = \exp[A_i + A_i/V_i + T B_i]$$

COEFFICIENTS IN THE EQUATIONS

P/MPa	A ₁ /K	A ₂ /K ²	A ₃ /K	A ₄ /K ²
101.32	248.13	0	-46.874	0
	(28.2)	(0)	(12.7)	(0)

The standard deviation (σ_{ij}) of the coefficients a_{ij} are given in parentheses.

P/MPa	A ₁	B ₁	C ₁	A ₂	B ₂	C ₂
101.32	14.24546	-2662.74	-53.46	13.92295	-3089.20	-65.29

Standard deviation (σ/T), relative standard deviation 100(ΔP/P), and absolute maximum deviation δ_{1,1}/K at P/MPa = 101.32 are resp.: 0.211, 0.728, 0.443.

AUXILIARY INFORMATION

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

Completions: The 27 T_{exp} data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies 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 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^s, ref. 6.

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

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