

Compiled by Thermodynamics Research Center

Components:	1. Ethyl acetate, $C_4H_8O_2$ [108-94-4] 2. 4-Propanol, C_3H_8O [71-23-4]
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
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)

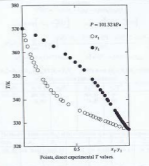
Editor(s) Skrzec, A.; Marczak, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

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), ref. 2

DIRECT EXPERIMENTAL VALUES

$P/P_0 = 101.32$					
x_1	T/K	y_1	x_2	T/K	y_2
0.000	379.29	0.000	0.582	334.37	0.085
0.014	367.48	0.126	0.607	333.82	0.092
0.038	365.35	0.209	0.640	333.28	0.100
0.067	362.78	0.295	0.662	332.78	0.106
0.078	359.38	0.406	0.686	332.36	0.112
0.088	357.81	0.458	0.715	331.79	0.120
0.104	355.87	0.499	0.731	331.43	0.124
0.121	354.26	0.543	0.779	330.72	0.136
0.141	352.58	0.583	0.805	330.28	0.143
0.151	348.62	0.660	0.825	329.86	0.149
0.210	347.29	0.686	0.851	329.43	0.155
0.229	345.90	0.710	0.875	328.98	0.160
0.265	344.17	0.736	0.913	328.47	0.173
0.287	343.00	0.756	0.932	327.69	0.186
0.319	341.74	0.777	1.008	327.29	1.000
0.357	340.14	0.798			
0.376	339.51	0.807			
0.426	338.06	0.829			
0.534	335.31	0.871			

Points, direct experimental T values.

AUXILIARY INFORMATION

Apparatus: The apparatus was a glass stillmanometer employing condenser circulation of the liquid and vapor phases with a charge capacity of 30 cm³, ref. 3. Turbidity mixing of the phases enabled equilibrium to be reached in a relatively short time. The stillmanometer was connected to a vacuum pump and a Fisher model VKE pressure controller. High purity nitrogen was used for the backing pressure. The temperatures were measured by a AISL-725 digital platinum resistance thermometer with a precision of readings ± 0.01 mK.

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-35 vibrating-tube digital densimeter with a precision of 0.02 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 compositions ≤ 0.005 mole fraction.

Materials:
1. Fluka AG (Buchs, St. Gallen, Switzerland), "pure" p.a. grade material, purity > 99.8 mole %; 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), "pure" p.a. grade material, purity > 99.8 mole %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.3833$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 798.54$; ref. 4.

Errors: $|t|/K = 0.02$; $|P/P_0| = 10$; $|x_1| = 0.005$; $|y_1| = 0.01$.

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Compiled by Thermodynamics Research Center

Components:	1. Ethyl methacrylate, $C_5H_8O_2$ (189-84-7) 2. 1-Propene, C_3H_6O (75-23-5)
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
Methods:	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, de table 26 Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

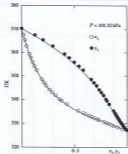
SOURCE OF DATA

Soto, 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); 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
0.08	339.29	0.0800
0.09	362.52	0.2901
0.16	356.46	0.4887
0.15	351.71	0.5841
0.26	347.95	0.6825
0.25	344.92	0.7179
0.36	342.46	0.7590
0.46	338.79	0.8156
0.50	335.96	0.8536
0.60	333.84	0.8825
0.70	332.07	0.9075
0.75	331.25	0.9197
0.80	330.46	0.9324
0.85	329.68	0.9458
0.90	328.89	0.9613
0.95	328.10	0.9787
1.00	327.29	1.0000

Standard deviation of T /K, relative standard deviation 100 $\Delta T/T$, and absolute maximum deviation Δy_i /K of y_i at P /Pa = 101.32 are resp. 0.135, 0.503, 0.348.



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

EQUATIONS

$$G^E(T) = -a_1 x_1 + a_2 x_2^2 - x_1 x_2 (c_1 + c_2 x_1)$$

$$v_i = \exp\left[-(a_i + \frac{b_i}{T})x_i\right] \quad v_2 = \exp\left[-(a_2 + \frac{b_2}{T})x_2\right]$$

$$P = P_1 + P_2 = \sum_{i=1}^2 v_i P_i^s \exp\left[\frac{v_i^L - G_i^L - v_i^G(P - P_i^s) - 2TP_i^s \Delta C_i - v_i^G}{RT}\right]$$

$$v_i^L = G^E - x_j \ln(G^E / (x_j v_j)) \quad v_i^G = G^E - x_j \ln(G^E / (x_j v_j))$$

$$B_{11}^E = B_{11} - B_{11}^L + B_{11}^G \quad B_{12}^E = B_{12} - B_{12}^L + B_{12}^G \quad B_{22}^E = B_{22} - B_{22}^L + B_{22}^G$$

COEFFICIENTS IN THE EQUATIONS

P/Pa	a_1 /K	a_2 /K ²	c_1 /K	c_2 /K ²
101.32	380.38	0	304.19	0
	0. 0	0.0	14. 0	0.0

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	14. 28445	-3054. 15	-26. 87	15. 83335	-3319. 65	-74. 29

AUXILIARY INFORMATION

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

Computations: The 34 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_{ij} , ref. 5, and the molar volumes under saturation pressure v_i^L , ref. 6.

Errors: Standard deviation $\sigma(T) = [2(T - T_{exp})^2]^{1/2} [36 + 2(1/T)^2]$
Relative standard deviation 100 $\sigma(T)/T$ = 100[2(σT)² / T_{exp}^2 + $(\sigma T)^2 / T^2]$
 N , number of experimental points, ref. 2.
 n , number of coefficients in the smoothing equation.

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HEAT CAPACITY OF LIQUIDS
SELECTED DATA ON MIXTURES
International DATA Series*
IN LIQUID-VAPOR EQUILIBRIUM

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

Compiled by Thermodynamics Research Center

Components: 1. 1-Propanol, C_3H_8O [71-23-9]
 2. Ethyl ethanoate, $C_4H_8O_2$ [75-66-4]

Status: 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, 35011 Las Palmas de Gran Canaria, Canary Islands, Spain)

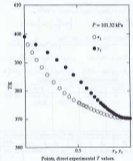
Edited by: Sliemers, A.; Moczydlowski, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

González, E.; 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

$P/101.32$																		
x_1	T/K	y_1	x_1	T/K	y_1													
0.0008	399.26 ^a	0.0000	0.0007	372.81	0.0204													
0.0316	396.45	0.1079	0.7229	372.38	0.0303													
0.0728	393.68	0.2183	0.7513	371.92	0.0401													
0.1144	391.07	0.3058	0.7818	371.57	0.0715													
0.1623	388.42	0.3886	0.8174	371.14	0.0850													
0.2133	385.75	0.4621	0.8517	370.83	0.1133													
0.2727	383.15	0.5361	0.8807	370.59	0.1302													
0.3292	381.04	0.5872	0.9143	370.51	0.1482													
0.3798	379.34	0.6300	0.9520	370.47	0.1720													
0.4285	378.05	0.6635	0.9660	370.40	0.1813													
0.4671	376.92	0.6928	1.0000	370.35	1.0000													
0.5160	375.94	0.7281																
0.5682	375.38	0.7235																
0.6432	375.21	0.7417																
0.5563	375.05	0.7369																
0.5795	374.65	0.7585																
0.5818	374.49	0.7666																
0.6282	373.80	0.7851																
0.6568	373.29	0.8019																



AUXILIARY INFORMATION

Apparatus: The apparatus was a glass ebulliometer employing continuous circulation of the liquid and vapor phases with a capacity of approx. 60 cm³; ref. 3. Turbulent mixing of the phases enabled equilibrium to be reached in a relatively short time. The ebulliometer was connected to a vacuum pump and the pressure controlled by a VakuumHEB electronic instrument (NOMACHHEB Gerätebau Wertheim) and measured with a mercury manometer.

Procedure: The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-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 < 0.001 mole fraction.

Materials: 1. Fluka AG (Buchs, St. Gallen, Switzerland); purity > 99 mol %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.3835$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 799.60$.

2. Fluka AG (Buchs, St. Gallen, Switzerland); purity > 99 mol %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.2626$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 875.89$; ref. 4.

Errors: $\pm 0.1 \text{ K}$; ± 0.01 ; ± 0.01 ; ± 0.01 ; ± 0.01 ; ± 0.02 .

REFERENCES

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3. Ortega, J.; Peña, J. A.; de Alfonso, C. *J. Chem. Eng. Data*, 1986, 31, 320.
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SELECTED DATA ON MIXTURES
International Data Series*
No. LIQUID-VAPOR EQUILIBRIUM

National Institute of Standards and Technology, Gaithersburg, MD 20899-7028

Compiled by Thermodynamics Research Center

Components: 1. 1-Propanol, C_3H_7O (71-23-6)
2. Butyl acetate, $C_6H_{12}O_2$ (72-26-0)
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 temperatures, 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, de table No. Universidad de Las Palmas de Gran Canaria, 35070 Las Palmas de Gran Canaria, Canary Islands, Spain)

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

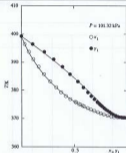
SOURCE OF DATA

Ortega, J.; 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

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

		P/MPa = 101.32					
x_1	T/K	y_1					
0.00	399.26	0.0000					
0.05	395.18	0.1524					
0.10	394.76	0.2718					
0.15	388.83	0.3600					
0.20	386.30	0.4477					
0.25	384.06	0.5167					
0.30	382.12	0.5719					
0.40	378.83	0.6647					
0.50	376.22	0.7368					
0.60	374.16	0.7908					
0.70	372.57	0.8432					
0.75	371.93	0.8650					
0.80	371.39	0.8859					
0.85	370.93	0.9069					
0.90	370.59	0.9293					
0.95	370.36	0.9572					
1.00	370.33	1.0000					

Smoothed deviation $\Delta T/K$, relative standard deviation 100 $\Delta T/T$, and absolute maximum deviation $\delta_a T/K$ at P/MPa = 101.32 are resp.: 0.134, 0.407, 0.290.



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

EQUATIONS

$$G^E/RT = -a_1x_1 + a_2x_2^2 - a_3x_1x_2 + a_4x_1^3$$

$$v_1 = \exp\left[-a_5x_1 + \frac{a_6}{RT}\right] \quad v_2 = \exp\left[-a_5x_2 + \frac{a_6}{RT}\right]$$

$$P = P_1^* + P_2^* \sum_{i=1}^2 x_i P_i^* \exp\left[\frac{P_1^* - (B_1 - P_1^*(P - P_1^*)) - 2P_1^* \sum_{i=1}^2 (B_i - P_i^*(P - P_i^*))}{RT}\right]$$

$$P_1^* = G^E - a_7(P/P^*)^2 \quad P_2^* = G^E - a_7(P/P^*)^2$$

$$B_1^* = B_1 - (B_1 + B_2)/2; \gamma_1 = P/P^*; P_1^*(x_1) = \exp\left[A_1 + B_1/(T + C_1) + 2B_2\right]$$

P/MPa	a_1/K	a_2/K^2	a_3/K	a_4/K^2
101.32	651.75 (18.2)	0	-308.10 (0.3)	8 00

The standard deviations (σ_{a_i}) of the coefficients a_i are given in parenthesis.

P/MPa	A_1	B_1	C_1	A_2	B_2	C_2
101.32	15.8049	-3304.67	-74.98	14.9679	-3876.54	-43.85

AUXILIARY INFORMATION

Measurements: The T_{exp} data at 101.32 kPa are reported in ref. 2.
Computations: The 30 T_{exp} data at 101.32 kPa were reduced using the modified Wilson equation, ref. 3, for the partial molar excess Gibbs energies, G_1^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 and/or saturation pressure P_i^* , 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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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

Component:	1. 3-Pyranol, $C_4H_6O_2$ (71-23-8) 2. Methyl propenoate, $C_4H_6O_2$ (199-01-2)
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
Parameter:	P , pressure
Method:	Direct measurement of T , x_i and y_i at constant P , ref. 1

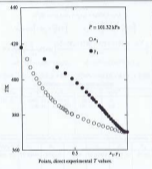
Author(s) of table:	Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 Las Palmas de Gran Canaria, Canary Islands, Spain)
Edited by:	Skowis, A.; Mącznyk, A. (Instytut Chemii Fizycznej, Polska Akademia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

SOURCE OF DATA

Gonzalez, E.; 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_1	T/K	y_1												
0.0080	410.26*	0.8000	0.4768	380.82	0.8079												
0.0535	411.82	0.2197	0.5325	379.20	0.8269												
0.0649	487.17	0.3404	0.5858	377.36	0.8484												
0.1128	483.72	0.4186	0.6327	376.48	0.8672												
0.1419	480.69	0.4869	0.6839	375.41	0.8856												
0.1687	398.19	0.5282	0.7304	374.46	0.8993												
0.1986	395.46	0.5778	0.7708	373.72	0.9119												
0.2380	393.16	0.6273	0.8154	372.93	0.9261												
0.2497	391.62	0.6428	0.8318	372.20	0.9387												
0.2771	389.85	0.6711	0.8669	371.51	0.9518												
0.2918	388.82	0.6869	0.9285	370.92	0.9652												
0.3172	387.56	0.7676	0.9524	370.49	0.9783												
0.3533	385.87	0.7372	0.9684	370.37	0.9791												
0.3753	384.43	0.7534	1.0000	370.35	1.0000												
0.3922	383.94	0.7688															
0.4073	383.18	0.7787															
0.4196	382.73	0.7794															
0.4326	381.89	0.7959															
0.4739	380.89	0.8020															



AUXILIARY INFORMATION

Apparatus:	The apparatus was a glass ebullioscope employing continuous circulation of the liquid and vapor phases with a capacity of around 60 cm ³ , 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 Yokogawa electronic instrument (Horusch&Gonzalez Wirthlich) and measured with a mercury manometer.
Procedure:	The procedure was described in ref. 3. The compositions were determined by measuring their densities at 298.15 K with an Anton Paar model DMA-35 vibrating-tube digital densimeter with a precision of ±0.02 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 < 0.001 mole fraction.
Materials:	1. Fluka AD (Buchs, St. Gallen, Switzerland), purity > 99 mol %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K}) = 1.3833$, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 799.80$. 2. Aldrich (Steinheim, Germany), purity 99+ mol %; degassed ultrasonically, dried over molecular sieves 3A; $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 871.12$, ref. 4.
Errors:	±0.7 K; ±0.03; ±0.01; ±0.005; ±0.01; ±0.03.

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

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

Compiled by Thermodynamics Research Center

Components: 1. 1-Propanol, C_3H_7O (71-23-8)
2. Methyl propanoate, $C_4H_8O_2$ (100-69-2)
States: 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 of variable x_1 and constant P , ref. 1

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

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

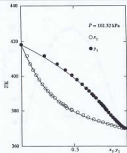
SOURCE OF DATA

González, E.; 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_1

P/Pa = 101.32		
x_1	T/K	y_1
0.00	418.26	0.0000
0.05	411.68	0.2033
0.10	405.49	0.3650
0.15	400.06	0.4870
0.20	395.43	0.5778
0.25	391.58	0.6409
0.30	388.58	0.6880
0.40	383.43	0.7719
0.50	379.85	0.8228
0.60	377.15	0.8605
0.70	375.03	0.8928
0.75	374.11	0.9078
0.80	373.26	0.9251
0.85	372.47	0.9391
0.90	371.73	0.9566
0.95	371.02	0.9764
1.00	370.31	1.0000

Standard deviation of T/K , relative standard deviations 100(dT/T)%, and absolute maximum deviation $\Delta_{max} T/K$ at P/Pa = 101.32 are resp.: 0.234, 0.792, 0.468.



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

EQUATIONS

$$G^E(T) = -x_1(z_1x_1 + v_1x_1^2) - x_2(z_2x_2 + v_2x_2^2)$$

$$v_1 = \exp\left[-(a_1 + \frac{b_1}{T})\right] \quad v_2 = \exp\left[-(a_2 + \frac{b_2}{T})\right]$$

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

$$P_i^L = G^E - v_i f_i G^E(T, z_i, v_i)_{T,P} \quad P_i^V = G^E - v_i f_i G^E(T, z_i, v_i)_{T,P}$$

$$B_{ii}^L = B_{ii}^{L,0} - (B_{ii}^L - B_{ii}^{L,0})^2 \cdot y_i = P_i^L / P_i^V \quad P_i^L/P_i^V = \exp\left[A_i + B_i/T + C_i/T^2\right]$$

COEFFICIENTS IN THE EQUATIONS

P/Pa	a_i/K	b_i/K^2	c_i/K	d_i/K^2
101.32	-2462.22 (330.4)	101800 (43392)	36.367 (40.4)	9 (0)

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

P/Pa	A_i	B_i	C_i	D_i	E_i
101.32	15.80449	-3.06647	-18.98	13.47578	-2837.50

AUXILIARY INFORMATION

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

Computations: The 53 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 equations parameters were taken from refs 4 and 5, 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. 6, and the molar volumes under saturation pressure V_i^L , ref. 7.

Errors: Standard deviation of T = $[2(17 - T_{exp})^2 / (N - 2)]^{1/2}$,
Relative standard deviation 100(dT/T)% = $100[2(17 - T_{exp})^2 / (N - 2)]^{1/2}$,
 N , number of experimental points, ref. 2,
 n , number of coefficients in the smoothing equation.

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Compiled by Thermodynamic Research Center

Components: 1. Ethyl methanoate, C₂H₄O₂ (109-94-0)
2. 1-Propanol, C₃H₇O (77-23-8)

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

Variables: V^E, molar excess volume
x₁, 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 x₁; 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: Slawski, A.; Moczyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

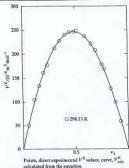
Soto, A.; Hernández, P.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Note: P = 101.32 kPa.

TK = 298.15

x ₁	V ^E /10 ⁻⁶ m ³ mol ⁻¹						
0.0124	39						
0.1134	105						
0.1554	134						
0.1964	160						
0.2394	177						
0.3014	212						
0.3546	227						
0.4052	240						
0.4480	245						
0.4911	246						
0.5146	248						
0.5941	257						
0.6538	259						
0.6976	268						
0.7500	178						
0.7754	169						
0.8372	138						
0.8821	100						
0.9205	59						



SMOOTHING EQUATION

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

Coefficients a_i in the smoothing equation, standard deviation s_d, and maximum deviation s_m determined by least-squares analysis.

TK	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆	s _d	s _m
	R ² /mol ⁻¹							
298.15	987.0 (2.6)	-39.7 (6.9)					2.2	4.5

The standard deviations (s_d) of the coefficients a_i are given in parentheses. s_d = max{|(a_i - V^E)/V^E|}; s_m = [210⁶ s_d - V^E]/N. 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 ±0.01 K with a flow-thermostat.

Procedure: The procedure was described in ref. 1. Mixtures were prepared by weighing in hermetically sealed 2.5 cm³ 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 ethanolicity, dried over molecular sieves 3A; w₁ 298.15 K = 1.3576, ρ(298.15 K) kg m⁻³ = 914.93; T_b(101.32 kPa)°K = 327.29.
2. Fluka AG (Buchs, St. Gallen, Switzerland), "specios p.a." grade material, purity > 99.8 mole %; degassed ethanolicity, dried over molecular sieves 3A; w₁ 298.15 K = 1.3835, ρ(298.15 K) kg m⁻³ = 799.54; ref. 4; T_b(101.32 kPa)°K = 370.29.

Notes: JTK = 0.02, s_d = 0.0005, s_m = 10⁻⁶ m³ mol⁻¹ < 3.

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SELECTED DATA ON MIXTURES
International Data Series*

3a. EXCESS VOLUME

National Institute of Standards and Technology, Boulder, CO 80505-3303

Compiled by Thermodynamics Research Center

Components: 1. 1-Propanol, C₃H₈O [77-25-2]
2. Butyl methacrylate, C₉H₁₈O₂ [392-54-7]
State: Binary system, single-phase liquid, pure components, both liquid
Variables: V^E, molar excess volume
x₁, mole fraction of component 1
Parameters: Z, temperature
Constants: P, pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x₁; ref. 1

Author(s): Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, 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)

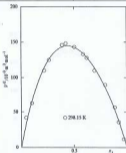
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González, E.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: P = 101.325 kPa.

TK = 298.15					
x ₁	V ^E /10 ⁻³ m ³ mol ⁻¹				
0.0457	42				
0.0995	63				
0.2162	119				
0.2632	125				
0.3673	146				
0.4251	148				
0.5050	143				
0.5880	133				
0.6212	128				
0.6860	119				
0.7970	90				
0.8865	57				
0.9226	36				
0.9763	12				



SMOOTHING EQUATION

$$V_{\text{calc}}^E = x_1 x_2 \sum_{i=0}^5 a_i (x_1 - x_2)^i$$

Coefficients a_i in the smoothing equation, standard deviation σ_a, and maximum deviation δ_m determined by least-squares analysis.

TK	a ₁	a ₂	a ₃	a ₄	a ₅	σ _a	δ _m
	m ³ mol ⁻¹						
298.15	572.2 (7.6)	-122.2 (16.4)	96 (35)			4.0	8.8

The standard deviation σ_a of the coefficients a_i are given in parentheses
δ_m = max |V^E_{calc} - V^E|; σ_a = [20/(N - 6)]^{1/2} ∑ (V^E_{calc} - V^E)² / (N - 6)^{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 ±0.02 kg m⁻³. The temperature was controlled at ±0.01 K with a Heto ultrathermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5-cm³ 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. Pthko AG (Basel, St. Gallen, Switzerland), purity > 99 mol-%; degassed ultrasonically, dried over molecular sieves 3A; ρ(298.15 K) = 1.3835, ρ(298.15 K)/kg m⁻³ = 799.60, T_g(101.32 kPa)/K = 370.35.
2. Aldrich (Steinheim, Germany), purity 97+ mol-%; degassed ultrasonically, dried over molecular sieves 3A; ρ(298.15 K) = 1.3872, ρ(298.15 K)/kg m⁻³ = 857.64, T_g(101.32 kPa)/K = 379.39; ref. 4.

Error: δTK = 0.02; δx₁ = 0.0003; δV^E/10⁻³ m³mol⁻¹ < 4.

REFERENCES

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3. Ortega, J.; Mateo, J. S.; Paz-Andrade, M. I.; Jiménez, E. *J. Chem. Thermodyn.*, 1993, 25, 1127.
4. González, E.; Ortega, J. *J. Chem. Eng. Data*, 1999, 40, 1178.

Compiled by Thermodynamics Research Center

Component: 1. 1-Propanol, C_3H_8O (71-23-8)
 2. Ethyl ethanoate, $C_4H_8O_2$ (121-65-4)
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) 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: Skrzut, A., Maczynski, A. (Instytut Chemii Przemysłowej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

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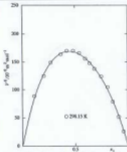
González, E.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 2

DIRECT EXPERIMENTAL VALUES

Note: $P = 101.32$ kPa

TK = 298.15

x_1	$V^E/10^{-6}$ $m^3 \text{mol}^{-1}$								
0.1028	89								
0.2017	125								
0.2685	149								
0.3656	164								
0.4232	170								
0.4849	170								
0.5413	166								
0.5989	156								
0.6397	148								
0.6861	138								
0.7465	124								
0.8065	105								
0.8591	79								
0.9129	52								
0.9579	26								



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

SMOOTHING EQUATION

$$V^E_{\text{calc}} = a_1 x_1 + a_2 \sum_{i=1}^n (x_1 - x_2)^{2i+1}$$

Coefficients a_i in the smoothing equation, standard deviation σ_{ij} , and maximum deviation Δ_{max} determined by least-squares analysis.

TK	a_1	a_2	a_3	a_4	a_5	a_6	Δ_{max}
	298.15	671.3 (4.2)	-116.9 (9.6)	147 (30)			2.4

The standard deviations σ_{ij} of the coefficients a_i are given in parentheses
 $\Delta_{\text{max}} = \max |V^E_{\text{calc}} - V^E|$; $\sigma_{ij} = [20 \sum_{i=1}^n (V^E_{\text{calc}} - V^E)^2 / (N - i)]^{1/2}$
 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 ± 0.01 K with a Heto ultrathermostat.

Procedure: The procedure was described in ref. 1. Mixtures were prepared by weighing in hermetically sealed 25 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), purity > 99 mol-%; degassed ultrasonically, dried over molecular sieves 3A; $w(1)$, 298.15 K) = 1.3031, $\rho(298.15 \text{ K})/\text{kg m}^{-3}$ = 799.50, $T_f(101.32 \text{ kPa})/\text{K}$ = -77.35.
 2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mol-%; degassed ultrasonically, dried over molecular sieves 3A; $w(2)$, 298.15 K) = 1.3920, $\rho(298.15 \text{ K})/\text{kg m}^{-3}$ = 875.89, $T_f(101.32 \text{ kPa})/\text{K}$ = 39.26, ref. 4.

Error: $\Delta T/K = 0.02$; $\Delta \rho_i = 0.0005$; $\Delta V^E/10^{-6} \text{ m}^3 \text{mol}^{-1} < 4$.

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- Ortega, J.; Matos, J. S.; Paz-Antuñedo, M. I.; Sandoz, E. *J. Chem. Thermodyn.*, 1986, 17, 1127.
- González, E.; Ortega, J. *J. Chem. Eng. Data*, 1995, 46, 1178.

Compiled by Thermodynamics Research Center

Components:	1. <i>n</i> -Propyl, C_3H_7O (73-23-6) 2. Methyl propionate, $C_5H_8O_2$ (298-61-2)
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: Stroncz, A.; Maryczki, A. Gwydzia Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

SOURCE OF DATA

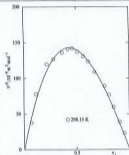
González, E.; Ortega, J. Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain); ref. 1

DIRECT EXPERIMENTAL VALUES

Notes: $P = 101.325$ kPa.

TR: = 298.15

x_1	$V^E/10^{-6}$ $m^3 \cdot mol^{-1}$						
0.0669	38						
0.1131	78						
0.2398	120						
0.2841	127						
0.3656	136						
0.4318	141						
0.4639	142						
0.5129	137						
0.5676	131						
0.6140	124						
0.6797	109						
0.7875	89						
0.8872	77						
0.8515	60						
0.9068	39						
0.9305	23						



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

SMOOTHING EQUATION

$$V^E_{calc} = a_1 + a_2 \sum_{i=1}^n (x_i - x_j)^{1/2}$$

Coefficients a_i in the smoothing equation, standard deviation s_m , and maximum deviation δ_m , determined by least-squares analysis.

TR	a_1	a_2	a_3	a_4	a_5	a_6	δ_m
	$m^3 \cdot mol^{-1}$						
298.15	562.5 (8.0)	-152.0 (16.7)				4.5	8.9

The standard deviations (only) of the coefficients a_i are given in parentheses. $\delta_m = \max |V^E_{calc} - V^E|$; $s_m = [2 \sum (V^E_{calc} - V^E)^2 / (N - 6)]^{1/2}$. 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 ± 0.02 kg m^{-3} . The temperature was controlled at ± 0.01 K with a Teco thermostat.

Procedure: The procedure was described in ref. 3. Mixtures were prepared by weighing in hermetically sealed 2.5 cm³ 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 AG (Buchs, St. Gallen, Switzerland), purity > 99 mol %; degassed ultrasonically, dried over molecular sieves 3A; $d(298.15 \text{ K}) = 1.3835$, $\rho(298.15 \text{ K}) \text{ kg} \cdot \text{m}^{-3} = 799.60$, $T_f(101.32 \text{ kPa}) \text{ K} = 370.35$.
2. Aldrich (Steinheim, Germany), purity 99+ mol %, degassed ultrasonically, dried over molecular sieves 3A; $d(298.15 \text{ K}) = 1.3069$, $\rho(298.15 \text{ K}) \text{ kg} \cdot \text{m}^{-3} = 871.12$, $T_f(101.32 \text{ kPa}) \text{ K} = 438.26$; ref. 4.

Errors: ± 0.02 ; $\delta_1 = 0.0002$; $dV^E/10^{-6} m^3 \cdot mol^{-1} < 4$.

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- González, E.; Ortega, J. *J. Chem. Eng. Data*, 1998, 40, 1178.

Compiled by Thermodynamics Research Center

Components:	1. 1-Propanol, C ₃ H ₈ O [77-27-0] 2. Benzyl Isocyanate, C ₉ H ₉ N [209-21-7]
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
Methods:	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:	Stancu, A.; Młyński, A. (Instytut Chemii Fizycznej, Polska Akademia Nauk, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland)

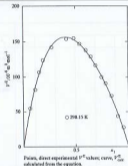
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Guadalupe, E.; Ortega, J. (Laboratorio de Termodinámica y Fisicoquímica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, Canary Islands, Spain), ref. 2

DIRECT EXPERIMENTAL VALUES

Notes: $P = 101.32$ kPa.

TK = 298.15						
x_1	$V^E/10^3$ $\text{m}^3 \text{mol}^{-1}$					
0.0051	55					
0.0136	82					
0.0316	107					
0.0887	128					
0.2706	142					
0.4139	154					
0.4849	155					
0.5389	147					
0.5978	138					
0.6457	129					
0.6993	117					
0.7465	100					
0.7840	91					
0.8393	75					
0.8978	44					
0.9300	35					



SMOOTHING EQUATION

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

Coefficients a_j in the smoothing equation, standard deviation σ_j , and maximum deviation δ_{max} determined by least-squares analysis.

TK	a_1	a_2	a_3	a_4	a_5	a_6	δ_{max}
	10^3 $\text{m}^3 \text{mol}^{-1}$						
298.15	606.7 (4.6)	-337.0 (8.8)	135.0 (19.1)				2.5 4.4

The standard deviations σ_j of the coefficients a_j are given in parentheses
 $\delta_{\text{max}} = \max |V^E_{\text{calc}} - V^E|$; $\sigma_j = [2(V^E_{\text{calc}} - V^E)^2 / (N - 6)]^{1/2}$
 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 ± 0.02 kg m ⁻³ . The temperature was controlled at ± 0.01 K with a Hele atmosphere.
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 acetone. A polynomial equation was used for describing the density-concentration curve.
Materials:	1. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mol %, degassed ultrasonically, dried over molecular sieves 3A; $n_D(298.15 \text{ K}) = 1.3435$, $\rho(298.15 \text{ K}) \text{ kg m}^{-3} = 799.60$, $T_f(101.32 \text{ kPa}) \text{ K} = 376.33$. 2. Fluka AG (Buchs, St. Gallen, Switzerland), purity > 99 mol %, degassed ultrasonically, dried over molecular sieves 3A; $n_D(298.15 \text{ K}) = 1.4845$, $\rho(298.15 \text{ K}) \text{ kg m}^{-3} = 864.87$, $T_f(101.32 \text{ kPa}) \text{ K} = 438.13$, ref. 4.
Errors:	$\delta TK = 0.02$, $\delta \rho_1 = 0.0002$, $\delta V^E = 16^{-6} \text{ m}^3 \text{mol}^{-1} < 3$.

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87

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