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Excess Volumes of Some Binary Mixtures Containing
Chlorobenzene

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(Department of Chemistry, University of North Texas,
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SELECTED DATA ON MIXTURES

International DATA Series

Ser. A. Thermodynamic Properties of Non-reacting Binary Systems of Organic Substances

Volume **1992**, No. 1, pages 45-49

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Chlorobenzene

W. E. Acree Jr.[●] and I-L. Teng

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FIRST PUBLISHED RESULTS

2c. Excess volume, pp. 45-49

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SELECTED DATA ON MIXTURES
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2c. EXCESS VOLUME

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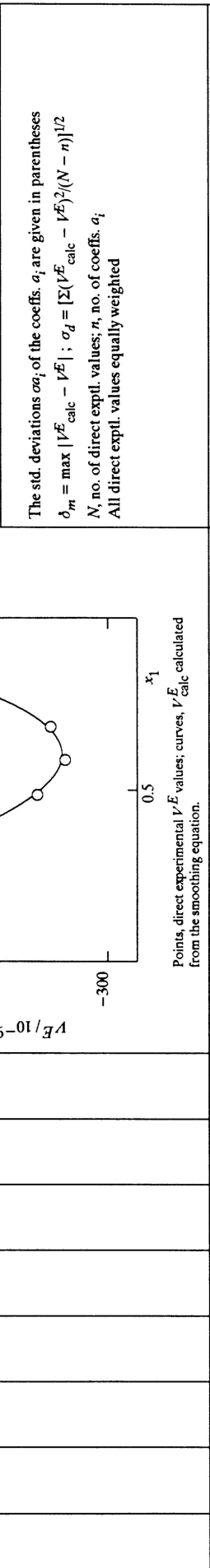
Published by Thermodynamics Research Center
Components: 1. Chlorobenzene, C₆H₅Cl
 2. Heptane, C₇H₁₆
State: Binary system, single-phase liquid; pure components, both liquid
Variables: V^E, molar excess volume
 x₁, mole fraction of component 1
Parameters: T, temperature
Constants: P, pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x₁; ref. 1

Author(s): Acree Jr., W. E. (Department of Chemistry, University of North Texas, Denton, TX 76203-5068, USA); Teng, I.-L.
Edited by: Kehiaian, H. V. (Institut de Topologie et de Dynamique des Systèmes, Université Paris VII, CNRS, 1, Rue Guy de la Brosse, 75005 Paris, France)

SOURCE OF DATA
 Acree Jr., W. E.; Teng, I.-L. (Department of Chemistry, University of North Texas, Denton, TX, USA); FIRST PUBLISHED RESULTS

DIRECT EXPERIMENTAL VALUES

Notes: P, atm.		SMOOTHING EQUATION						
T/K = 298.15		$V_{\text{calc}}^E = x_1 x_2 \sum_{i=1}^n a_i (x_1 - x_2)^{i-1}$						
x ₁		Coeffs. a _i in the smoothing eq., std. deviation σ _d and max. deviation δ _m detd. by least-squares anal.						
0.1455	-68	a ₁	a ₂	a ₃	a ₄	a ₅	σ _d	δ _m
0.2709	-140	10 ⁻⁹ m ³ mol ⁻¹						
0.3856	-204							
0.4875	-252							
0.5891	-271							
0.6841	-261							
0.7672	-218							
0.8462	-177							
0.9245	-96							



AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter (Anton Paar, Graz, Austria), model DMA 55, equipped with a thermostating water bath (Neslab Instruments, Portsmouth, NH, USA). Temp. was controlled to within 0.005 K and was measured by means of a Beckman thermometer (Beckman Instruments, Inc., Fullerton, CA, USA) which was periodically compared against a calibrated (National Bureau of Stds., USA) Pt-resistance thermometer. Samples were introduced by means of a glass syringe.

Procedure: Density, ρ, was calcd. from period of vibration, τ; ρ = a + bτ². Consists. a and b were detd. by calibrating the app. with benzene, ρ(298.15 K)/kg m⁻³ = 873.63, doubly distd. and degassed water ρ(298.15 K)/kg m⁻³ = 997.04, and cyclohexane ρ(298.15 K)/kg m⁻³ = 773.85. Mixts. were prepd. by weighing. V^E was calcd. from V^E = V - (x₁V₁⁰ + x₂V₂⁰), where V = (x₁M₁ + x₂M₂)/ρ is the molar vol. of the mixt. and V_i⁰ = V(x_i = 1) and M_i are, resp., the molar vol. and the molar mass of component i.

Materials: 1. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; ρ₁(298.15 K)/kg m⁻³ = 1101.98; M₁/10⁻³ kg mol⁻¹ = 112.5584.
 2. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99 mole %, stored over mol. sieves and used without further purification. Purity tested by GLC, > 99.8 mole %; ρ₂(298.15 K)/kg m⁻³ = 679.55; M₂/10⁻³ kg mol⁻¹ = 100.20404.

Errors: δT (reproducibility)/K < 0.003; δT/(TPTS-68)/K = 0.01; δx₁ = 0.0001; δV^E/10⁻⁹ m³ mol⁻¹ < 20.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 2c, 1979.*

Components: 1. Chlorobenzene, C₆H₅Cl
2. Octane, C₈H₁₈
Binary system, single-phase liquid; pure components, both liquid

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

Variables: V^E , molar excess volume

Parameters: x_i , mole fraction of component i
 T , temperature

Constants: P , pressure

Method: Calculation of V^E from density measurements at constant T and P and variable x_i ; ref. 1

Author(s): Acree Jr., W. E. (Department of Chemistry, University of North Texas, Denton, TX 76203-5068, USA); Teng, I.-L.

Edited by: Kehiaian, H. V. (Institut de Topologie et de Dynamique des Systèmes, Université Paris VII, CNRS, 1, Rue Guy de la Brosse, 75005 Paris, France)

SOURCE OF DATA
Acree Jr., W. E.; Teng, I.-L. (Department of Chemistry, University of North Texas, Denton, TX, USA); FIRST PUBLISHED RESULTS

DIRECT EXPERIMENTAL VALUES

Notes: P , atm.	
T/K	298.15
x_1	0.1595 0.2920 0.4130 0.5119 0.6127 0.7082 0.7879 0.8630 0.9340

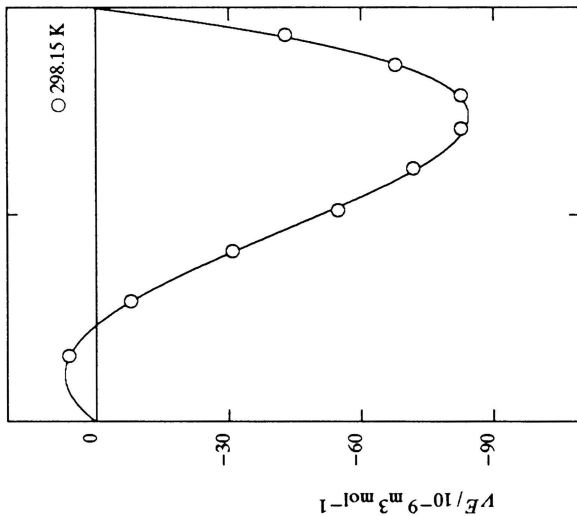
SMOOTHING EQUATION

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

Coeffs. a_i in the smoothing eq., std. deviation σ_d , and max. deviation δ_m detd. by least-squares anal.

T/K	a_1	a_2	a_3	a_4	a_5	σ_d	δ_m
298.15	-202.5 (2.8)	-439.7 (5.7)	-114 (13)			1.2	1.8

The std. deviations σ_d of the coeffs. a_i are given in parentheses
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$; $\sigma_d = [\sum (V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$
 N , no. of direct exptl. values; n , no. of coeffs. a_i
All direct exptl. values equally weighted



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

AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter (Anton Paar, Graz, Austria), model DMA 55, equipped with a thermostating water bath (Neslab Instruments, Portsmouth, NH, USA). Temp. was controlled to within 0.005 K and was measured by means of a Beckman thermometer (Beckman Instruments, Inc., Fullerton, CA, USA) which was periodically compared against a calibrated (National Bureau of Standards, USA) Pt-resistance thermometer. Samples were introduced by means of a glass syringe.

Procedure: Density, ρ , was calcd. from period of vibration, τ ; $\rho = a + b\tau^2$. Consists. a and b were detd. by calibrating the app. with benzene, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.63$, doubly distd. and degassed water, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 997.04$, and cyclohexane, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 773.85$. Mixts. were prepd. by weighing. V^E was calcd. from $V^E = V - (x_1 V_1^* + x_2 V_2^*)$, where $V = (x_1 M_1 + x_2 M_2) / \rho$ is the molar vol. of the mixt. and $V_i^* = V(x_i = 1)$ and M_i are, resp., the molar vol. and the molar mass of component i .

Materials: 1. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; $\rho_1(298.15 \text{ K})/\text{kg m}^{-3} = 1101.98$; $M_1/10^{-3} \text{ kg mol}^{-1} = 112.5584$.
2. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) anhydrous material of stated purity > 99 mole %, stored over mol. sieves and used without further purification. Purity tested by GLC, > 99.8 mole %; $\rho_2(298.15 \text{ K})/\text{kg m}^{-3} = 698.61$; $M_2/10^{-3} \text{ kg mol}^{-1} = 114.23092$.

Errors: δT (reproducibility)/K < 0.003; δT (IPTS-68)/K = 0.01; $\delta x_1 = 0.0001$; $\delta V^E/10^{-9} \text{ m}^3 \text{ mol}^{-1} < 2.0$.

REFERENCES
1. *Int. DATA Ser., Ser. A, Guideline 2c, 1979.*

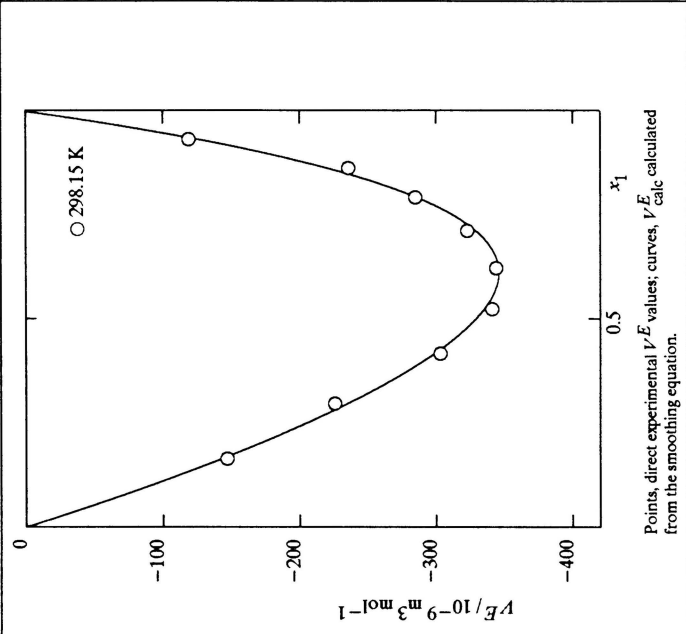
Author(s): Acree Jr., W. E. (Department of Chemistry, University of North Texas, Denton, TX 76203-5068, USA); Teng, I.-L.
Edited by: Kehiaian, H. V. (Institut de Topologie et de Dynamique des Systèmes, Université Paris VII, CNRS, 1, Rue Guy de la Brosse, 75005 Paris, France)

Components: 1. Chlorobenzene, C₆H₅Cl
 2. 2,2,4-Trimethylpentane, C₈H₁₈
State: Binary system, single-phase liquid; pure components, both liquid
Variables: V^E, molar excess volume
 x_i, mole fraction of component *i*
Parameters: T, temperature
Constants: P, pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x_i; ref. 1

SOURCE OF DATA
 Acree Jr., W. E.; Teng, I.-L. (Department of Chemistry, University of North Texas, Denton, TX, USA); FIRST PUBLISHED RESULTS

DIRECT EXPERIMENTAL VALUES

Notes: P, atm.	
T/K	298.15
x ₁	V ^E /10 ⁻⁹ m ³ mol ⁻¹
0.1632	-147
0.2983	-226
0.4174	-303
0.5243	-341
0.6217	-344
0.7108	-323
0.7910	-285
0.8621	-236
0.9309	-119



SMOOTHING EQUATION

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

Coeffs. a_i in the smoothing eq., std. deviation σ_d and max deviation δ_m detd. by least-squares anal.

T/K	a ₁	a ₂	a ₃	a ₄	a ₅	σ _d	δ _m
298.15	-1316 (22)	-577 (44)		-255 (100)		9.2	14

The std. deviations σ_d of the coeffs. a_i are given in parentheses
 δ_m = max |V^E_{calc} - V^E| ; σ_d = [Σ(V^E_{calc} - V^E)² / (N - n)]^{1/2}
 N, no. of direct exptl. values; n, no. of coeffs. a_i
 All direct exptl. values equally weighted

AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter (Anton Paar, Graz, Austria), model DMA 55, equipped with a thermostating water bath (Neslab Instruments, Portsmouth, NH, USA). Temp. was controlled to within 0.005 K and was measured by means of a Beckman thermometer (Beckman Instruments, Inc., Fullerton, CA, USA) which was periodically compared against a calibrated (National Bureau of Stds., USA) Pt-resistance thermometer. Samples were introduced by means of a glass syringe.

Procedure: Density, ρ, was calcd. from period of vibration, τ: ρ = a + bτ². Consts. a and b were detd. by calibrating the app. with benzene, ρ(298.15 K)/kg m⁻³ = 873.63, doubly distd. and degassed water ρ(298.15 K)/kg m⁻³ = 997.04, and cyclohexane ρ(298.15 K)/kg m⁻³ = 773.85. Mixts. were prepd. by weighing. V^E was calcd. from V^E = V - (x₁V¹ + x₂V²), where V = (x₁M₁ + x₂M₂)/ρ is the molar vol. of the mixt. and Vⁱ = V(x_i = 1) and M_i are, resp., the molar vol. and the molar mass of component *i*.

Materials: 1. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; ρ₁(298.15 K)/kg m⁻³ = 1101.98; M₁/10⁻³kg mol⁻¹ = 112.5584.
 2. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.7 mole %, stored over mol. sieves and used without further purification. Purity tested by GLC, > 99.8 mole %; ρ₂(298.15 K)/kg m⁻³ = 687.91; M₂/10⁻³kg mol⁻¹ = 114.23092.

Errors: δT (reproducibility)/K < 0.003; δT (IPTS-68)/K = 0.01; δx₁ = 0.0001; δV^E/10⁻⁹m³mol⁻¹ < 20.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 2c, 1979.*

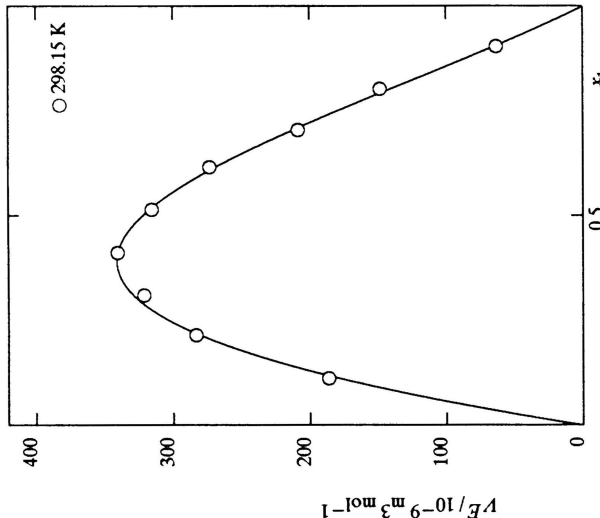
Components: 1. Chlorobenzene, C_6H_5Cl
2. Cyclohexane, C_6H_{12}
State: Binary system, single-phase liquid; pure components, both liquid
Variables: V^E , molar excess volume
 x_i , mole fraction of component i
Parameters: T , temperature
Constants: P , pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x_i ; ref. 1

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SOURCE OF DATA
Acree Jr., W. E.; Teng, I.-L. (Department of Chemistry, University of North Texas, Denton, TX, USA); FIRST PUBLISHED RESULTS

DIRECT EXPERIMENTAL VALUES

Notes: P , atm.	
$T/K = 298.15$	
x_1	$V^E/10^{-9} \text{ m}^3 \text{ mol}^{-1}$
0.1123	186
0.2139	283
0.3105	321
0.4108	340
0.5150	315
0.6169	273
0.7052	208
0.8036	148
0.9054	63



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

SMOOTHING EQUATION

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

Coeffs. a_i in the smoothing eq., std. deviation σ_d and max. deviation δ_m , detd. by least-squares anal.

T/K	a_1	a_2	a_3	a_4	a_5	σ_d	δ_m
298.15	1289.4 (9.7)	-649 (26)				5.6	7.7

The std. deviations σ_d ; of the coeffs. a_i are given in parentheses
 $\delta_m = \max |V^E_{\text{calc}} - V^E|$; $\sigma_d = [\Sigma(V^E_{\text{calc}} - V^E)^2 / (N - n)]^{1/2}$
 N , no. of direct exptl. values; n , no. of coeffs. a_i
All direct exptl. values equally weighted

AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter (Anton Paar, Graz, Austria), model DMA 55, equipped with a thermostating water bath (Neslab Instruments, Portsmouth, NH, USA). Temp. was controlled to within 0.005 K and was measured by means of a Beckman thermometer (Beckman Instruments, Inc., Fullerton, CA, USA) which was periodically compared against a calibrated (National Bureau of Stds., USA) Pt-resistance thermometer. Samples were introduced by means of a glass syringe.
Procedure: Density, ρ , was calcd. from period of vibration, τ ; $\rho = a + b\tau^2$. Consts. a and b were detd. by calibrating the app. with benzene, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.63$, doubly distd. and degassed water $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 997.04$, and cyclohexane $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 773.85$. Mixts. were prepd. by weighing. V^E was calcd. from $V^E = V - (x_1 V_1^* + x_2 V_2^*)$, where $V = (x_1 M_1 + x_2 M_2) / \rho$ is the molar vol. of the mixt. and $V_i^* = V(x_i = 1)$ and M_i are, resp., the molar vol. and the molar mass of component i .
Materials: 1. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; $\rho_1(298.15 \text{ K})/\text{kg m}^{-3} = 1101.98$; $M_1/10^{-3} \text{ kg mol}^{-1} = 112.5584$.
2. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; $\rho_2(298.15 \text{ K})/\text{kg m}^{-3} = 773.85$; $M_2/10^{-3} \text{ kg mol}^{-1} = 84.16128$.
Errors: δT (reproducibility)/K < 0.003; δT (IPTS-68)/K = 0.01; $\delta x_1 = 0.00001$; $\delta(V^E/10^{-9} \text{ m}^3 \text{ mol}^{-1}) < 20$.

REFERENCES

1. *Int. DATA Ser., Ser. A, Guideline 2c, 1979.*

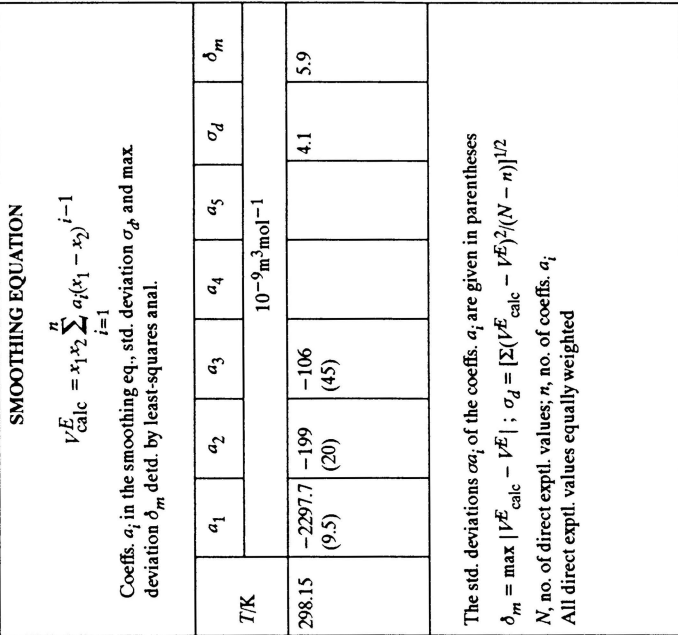
Components: 1. Chlorobenzene, C_6H_5Cl
2. Dibutyl ether, $C_8H_{18}O$
State: Binary system, single-phase liquid; pure components, both liquid
Variables: V^E , molar excess volume
 x_1 , mole fraction of component 1
Parameters: T , temperature
Constants: P , pressure
Method: Calculation of V^E from density measurements at constant T and P and variable x_1 ; ref. 1

Author(s): Acree Jr., W. E. (Department of Chemistry, University of North Texas, Denton, TX 76203-5068, USA); Teng, I.-L.
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SOURCE OF DATA
Acree Jr., W. E.; Teng, I.-L. (Department of Chemistry, University of North Texas, Denton, TX, USA); FIRST PUBLISHED RESULTS

DIRECT EXPERIMENTAL VALUES

Notes: P , atm.	
$T/K = 298.15$	
$V^E/10^{-9}$ $m^3 \cdot mol^{-1}$	
x_1	
0.1693	-309
0.3029	-473
0.4232	-559
0.5306	-571
0.6280	-548
0.7115	-492
0.7924	-409
0.8649	-291
0.9333	-156



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

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

Coeffs. a_i in the smoothing eq., std. deviation σ_d , and max. deviation δ_m detd. by least-squares anal.

T/K	a_1	a_2	a_3	a_4	a_5	σ_d	δ_m
298.15	-2297.7 (9.5)	-199 (20)	-106 (45)			4.1	5.9

The std. deviations σ_d of the coeffs. a_i are given in parentheses
 $\delta_m = \max |V_{calc}^E - V^E|$; $\sigma_d = [\sum (V_{calc}^E - V^E)^2 / (N - n)]^{1/2}$
 N , no. of direct exptl. values; n , no. of coeffs. a_i
All direct exptl. values equally weighted

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AUXILIARY INFORMATION

Apparatus: Vibrating tube densimeter (Anton Paar, Graz, Austria), model DMA 55, equipped with a thermostating water bath (Neslab Instruments, Portsmouth, NH, USA). Temp. was controlled to within 0.005 K and was measured by means of a Beckman thermometer (Beckman Instruments, Inc., Fullerton, CA, USA) which was periodically compared against a calibrated (National Bureau of Stds., USA) Pt-resistance thermometer. Samples were introduced by means of a glass syringe.

Procedure: Density, ρ , was calcd. from period of vibration, τ : $\rho = a + b\tau^2$. Consts. a and b were detd. by calibrating the app. with benzene, $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 873.63$, doubly distd. and degassed water $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 997.04$, and cyclohexane $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 773.85$. Mixts. were prepd. by weighing, V^E was calcd. from $V^E = V - (x_1 V_1^* + x_2 V_2^*)$, where $V = (x_1 M_1 + x_2 M_2) / \rho$ is the molar vol. of the mixt. and $V_i^* = V(x_i = 1)$ and M_i are, resp. the molar vol. and the molar mass of component i .

Materials: 1. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) HPLC grade material of stated purity > 99.9 mole %, stored over mol. sieves and used without further purification; $\rho(298.15 \text{ K})/\text{kg m}^{-3} = 1101.98$; $M_1/10^{-3} \text{ kg mol}^{-1} = 112.5584$.

2. Aldrich Chem. Co. Inc. (Milwaukee, WI, USA) anh. grade material of stated purity > 99 mole %, stored over mol. sieves and used without further purification. Purity tested by GLC, > 99.8 mole %. $\rho_2(298.15 \text{ K})/\text{kg m}^{-3} = 764.20$; $M_2/10^{-3} \text{ kg mol}^{-1} = 130.23032$.

Errors: δT (reproducibility)/K < 0.003; δT (PTS-68)/K = 0.01; $\delta x_1 = 0.0001$; $\delta V^E/10^{-9} \text{ m}^3 \text{ mol}^{-1} < 20$.