GONE0960

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Excess volumes of 12 binary liquid mixtures of propyl n-alkanoates (C4 - C7) + propan-2-ol, + butan-2-ol, or + 2-methylpropan-1-ol at 298.15 K

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The molar excess volumes V^E are reported at 298.15 K *for* 12 *binary liquid mixtures formed by four propyl n-alkanoates (methanoate, ethanoate, propanoate, and butanoate) with three alkanols (propan-2-ol, butan-2-ol, and 2-methylpropan-1-ol). All the V^E values are positive.*

1. INTRODUCTION

In continuation of our systematic experimental study [ORTJ0956] on the excess molar enthalpies H^E of 12 liquid mixtures containing a propyl n-alkanoate (methanoate, ethanoate, propanoate, or butanoate) and an alkan-2-ol (propan-2-ol or butan-2-ol) or an isoalkanol (2-methylpropan-1-ol), we present here molar excess volume, V^E, data at 298.15 K for the same 12 binary mixtures. The purpose of this investigation is to examine the effect of the molecular structure of isomeric alkanols on the properties of mixtures with n-alkanoates.

No data are found in the literature for the systems of this work.

2. EXPERIMENTAL SECTION

2.1. Apparatus and Procedure

A vibrating tube densimeter, Model DMA 55 (Anton Paar, Graz, Austria) was used. Temperature T was controlled to within 0.01 K using a Heto ultrathermostat and was measured by means of a calibrated digital precision thermometer DT 100-20 (Anton Paar, Graz, Austria) against ITS-90 to within $\sigma(T)$/K = 0.01.

Density, ρ, was calculated from period of vibration, τ:

$$\rho = a + b\tau^2 \qquad (1)$$

Constants a and b were determined by calibrating the apparatus with doubly distilled and degassed H_2O, ρ(298.15 K)/kg m^{-3} = 997.0474, [RIDJ0860], and nonane, ρ(298.15 K)/kg m^{-3} = 713.85, see [ORTJ0852]. Density measurements are taken with an accuracy of better than 0.01 kg m^{-3}. Mixtures were prepared by mass. V^E was calculated from ρ of the mixtures and the densities ρ_i and molar masses M_i of the pure components i:

$$V^E = V - (x_1M_1/\rho_1 + x_2M_2/\rho_2) \qquad (2)$$

$$V = (x_1M_1 + x_2M_2)/\rho \qquad (3)$$

The experimental uncertainties are $\sigma(x_1)$ = 0.0001 and $\sigma(V^E)/10^{-9}$m^{3}mol^{-1} = 2.

2.2. Materials

C_3H_8O, Propan-2-ol (Isopropanol) Fluka AG (Buchs, Switzerland) "puriss p.a." grade material of stated purity > 99.5 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.3751; ρ_i(298.15 K)/kg m^{-3} = 781.19.

$C_4H_8O_2$, Propyl methanoate (Propyl formate). Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.3744; ρ_i(298.15 K)/kg m^{-3} = 898.22.

$C_4H_{10}O$, Butan-2-ol (sec-Butanol). Fluka AG (Buchs, Switzerland) "puriss p. a." grade material of stated purity > 99.5 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.3953; ρ_i(298.15 K)/kg m^{-3} = 802.36.

$C_4H_{10}O$, 2-Methylpropan-1-ol (Isobutanol). Fluka AG (Buchs, Switzerland) "puriss p. a." grade material of stated purity > 99.5 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.3939; ρ_i(298.15 K)/kg m^{-3} = 797.83.

$C_5H_{10}O_2$, Propyl ethanoate (Propyl acetate). Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.3820; ρ_i(298.15 K)/kg m^{-3} = 882.18.

$C_6H_{12}O_2$, Propyl propanoate (Propyl propionate). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated purity > 99 mole % was degassed ultrasonically

and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.3908; ρ_i(298.15 K)/kg m^{-3} = 875.65.

$C_7H_{14}O_2$, Propyl butanoate (Propyl butyrate). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated purity > 99 mole % was degassed ultrasonically and dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.3976; ρ_i(298.15 K)/kg m^{-3} = 868.07.

3. RESULTS

The experimental V^E values of the 12 systems are tabulated and graphed in the Appendix and saved on disk as Standard ELDATA Files **GONE0960.001** through **GONE0960.012**.

The data were fitted to Eq. (1):

$$V^E_{calc}/\ m^3mol^{-1} = x_1x_2\Sigma A_i[x_1/(x_1 + kx_2)]^{i-1} \qquad (1)$$

all points weighted equally. With an adjusted coefficient k and n = 2 to 4 coefficients A_i the standard deviations $\sigma(V^E)$, defined by Eq.(2):

$$\sigma(V^E) = [\Sigma(V^E_{calc} - V^E)^2/(N-n)]^{1/2} \qquad (2)$$

where N is the number of experimental values, are less than 3.3 $10^{-9}m^3mol^{-1}$ (ca. 1 % at x_1 = 0.5).

4. DISCUSSION AND CONCLUSIONS

All the V^E values are positive with fairly symmetrical V^E vs. x_1 curves. The change of the equimolar V^E with the chain-length of the n-alkanoate, for a given alkanol, is less regular than in the case of H^E [ORTJ0956]. V^E decreases from the ethanoate to the propanoate, the butanoate having nearly the same V^E value as the propanoate.

REFERENCES

[ORTJ0852] – Ortega, J.; Matos, J. S.; Paz Andrade, M. I.; Jimenez, E. Excess molar volumes of (ethyl formate or ethyl acetate + an isomer of hexanol) at 298.15 K. *J. Chem. Thermodyn.* **1985,** *17,* 1127-1132.

[ORTJ0956] – Ortega, J.; Placido, J. Excess enthalpies of 12 binary mixtures of propyl alkanoates (C4 - C7) + propan-2-ol, + butan-2-ol, or + 2-methylpropan-1-ol at 298.15 K. *ELDATA Int. Electron. J. Phys.-Chem. Data* **1995,** *1,* 321-328.

[RIDJ0860] – Riddick, J. A.; Bunger, W. B.; Sakano, T. K. Techniques of Chemistry, Vol. II. *Organic Solvents, 4th Ed. John Wiley & Sons (ISBN 0-471-08467-0)* **1986,** 1-1325.

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Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.001**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

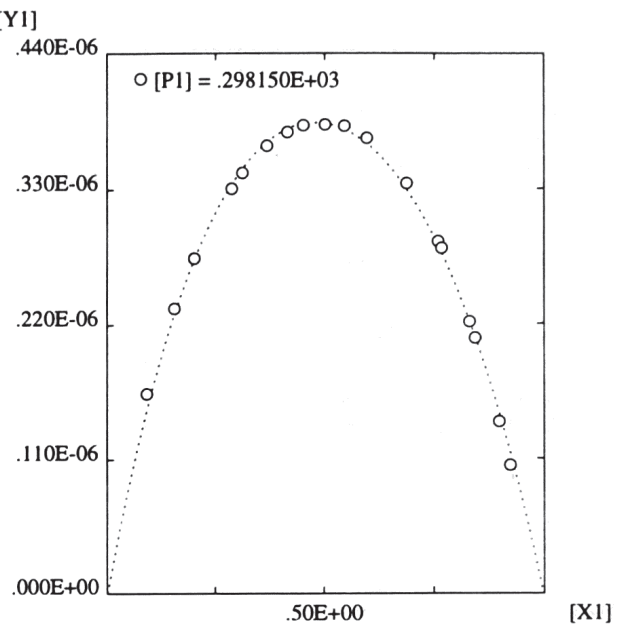
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. C_3H_8O , Propan-2-ol**
2. $C_4H_8O_2$, Propyl methanoate

[P1] = .298150E+03

[X1]	[Y1]
.933000E-01	.164200E-06
.156500E+00	.233600E-06
.202400E+00	.274400E-06
.288400E+00	.331100E-06
.314000E+00	.343300E-06
.368900E+00	.365400E-06
.416700E+00	.376600E-06
.451900E+00	.382000E-06
.502300E+00	.382400E-06
.545500E+00	.381300E-06
.597600E+00	.371400E-06
.687700E+00	.334600E-06
.760500E+00	.287200E-06
.768400E+00	.281800E-06
.832000E+00	.222100E-06
.844400E+00	.208600E-06
.899500E+00	.140300E-06
.924600E+00	.104900E-06



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State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

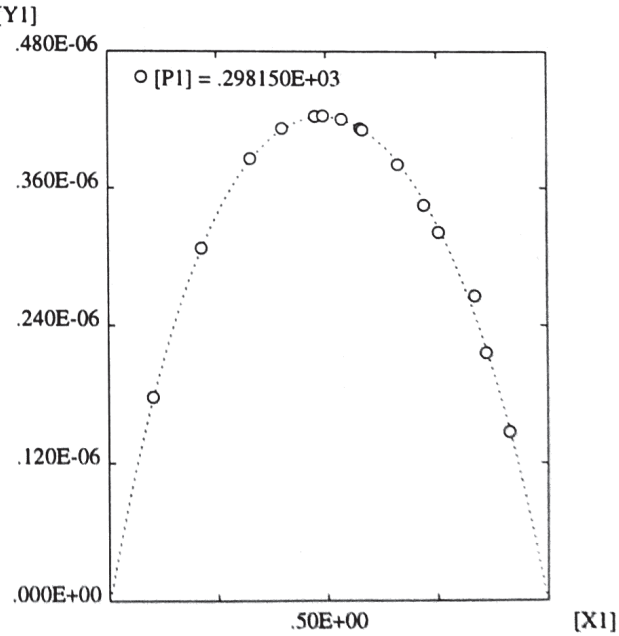
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. C_3H_8O , Propan-2-ol**
2. $C_5H_{10}O_2$, Propyl ethanoate

[P1] = .298150E+03

[X1]	[Y1]
.102300E+00	.177700E-06
.215200E+00	.308200E-06
.328100E+00	.386000E-06
.400200E+00	.412600E-06
.475600E+00	.423300E-06
.493900E+00	.423900E-06
.536400E+00	.421100E-06
.579300E+00	.412700E-06
.583600E+00	.411100E-06
.664000E+00	.380400E-06
.722700E+00	.345500E-06
.755200E+00	.322000E-06
.836400E+00	.265800E-06
.861000E+00	.216200E-06
.912900E+00	.147200E-06



Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.003**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume
Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. C_3H_8O , Propan-2-ol**
2. $C_6H_{12}O_2$, Propyl propanoate

[P1] = .298150E+03

[X1]	[Y1]
.474000E–01	.881000E–07
.495000E–01	.908000E–07
.122300E+00	.194000E–06
.244300E+00	.309300E–06
.252000E+00	.313800E–06
.290900E+00	.336800E–06
.344300E+00	.358200E–06
.433600E+00	.375800E–06
.496100E+00	.375000E–06
.537800E+00	.368700E–06
.607000E+00	.349300E–06
.680600E+00	.317800E–06
.755100E+00	.272600E–06
.814000E+00	.225600E–06
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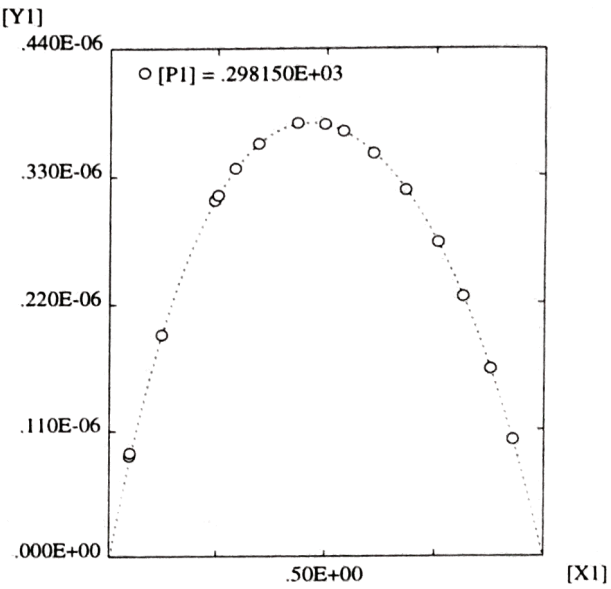
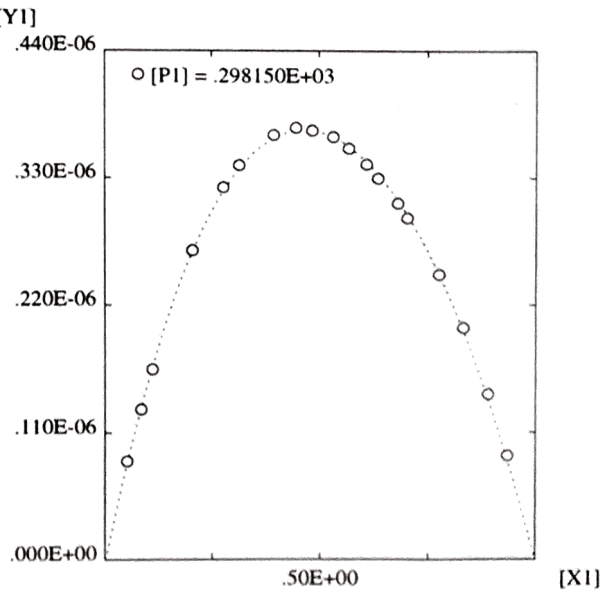


Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.004**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume
Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. C_3H_8O , Propan-2-ol**
2. $C_7H_{14}O_2$, Propyl butanoate

[P1] = .298150E+03

[X1]	[Y1]
.529000E–01	.853000E–07
.845000E–01	.130700E–06
.111500E+00	.165400E–06
.205100E+00	.267800E–06
.277300E+00	.322200E–06
.314100E+00	.341200E–06
.394200E+00	.367900E–06
.446100E+00	.373700E–06
.484200E+00	.371700E–06
.531500E+00	.365800E–06
.567500E+00	.356300E–06
.608100E+00	.342500E–06
.634900E+00	.330100E–06
.680000E+00	.308600E–06
.702300E+00	.295500E–06
.775100E+00	.246600E–06
.832400E+00	.200400E–06
.889900E+00	.143500E–06
.935700E+00	.900000E–07



Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.005**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_8O_2$, Propyl methanoate**
2. $C_4H_{10}O$, Butan-2-ol

[P1] = .298150E+03

[X1]	[Y1]
.687000E–01	.157200E–06
.821000E–01	.185100E–06
.114800E+00	.246700E–06
.205100E+00	.379500E–06
.231700E+00	.409800E–06
.287600E+00	.463100E–06
.335200E+00	.496000E–06
.390100E+00	.520900E–06
.447900E+00	.533200E–06
.490100E+00	.533100E–06
.560000E+00	.519600E–06
.580600E+00	.511300E–06
.624100E+00	.490000E–06
.707800E+00	.429600E–06
.808500E+00	.321100E–06
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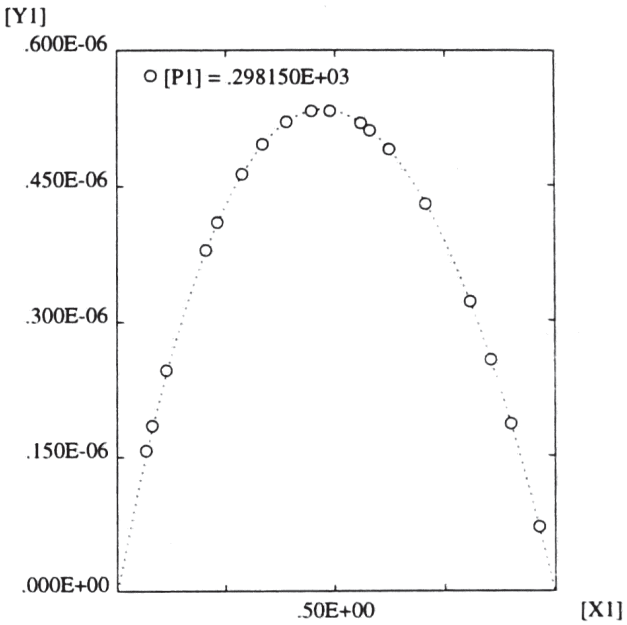

Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.006**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_8O_2$, Propyl methanoate**
2. $C_4H_{10}O$, 2-Methylpropan-1-ol

[P1] = .298150E+03

[X1]	[Y1]
.137600E+00	.141700E–06
.192600E+00	.184900E–06
.228200E+00	.208400E–06
.254700E+00	.224700E–06
.333100E+00	.261200E–06
.382800E+00	.276200E–06
.418500E+00	.284100E–06
.450900E+00	.287800E–06
.495500E+00	.289600E–06
.539700E+00	.286200E–06
.578400E+00	.279600E–06
.597500E+00	.275600E–06
.662200E+00	.254500E–06
.728400E+00	.224000E–06
.782400E+00	.191400E–06
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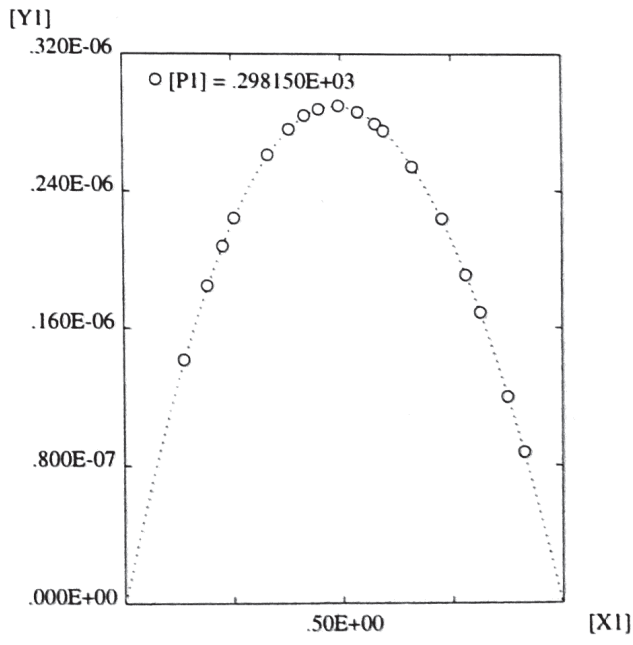
.913200E+00	.877000E–07



Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.007**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, Butan-2-ol**
2. $C_5H_{10}O_2$, Propyl ethanoate

[P1] = .298150E+03

[X1]	[Y1]
.940000E–01	.193900E–06
.145600E+00	.279800E–06
.187300E+00	.338800E–06
.209400E+00	.369600E–06
.289700E+00	.453700E–06
.326000E+00	.480700E–06
.353800E+00	.498500E–06
.423100E+00	.534100E–06
.476400E+00	.544900E–06
.553300E+00	.544700E–06
.608200E+00	.532700E–06
.679000E+00	.496800E–06
.718100E+00	.459700E–06
.770800E+00	.410800E–06
.788000E+00	.391600E–06
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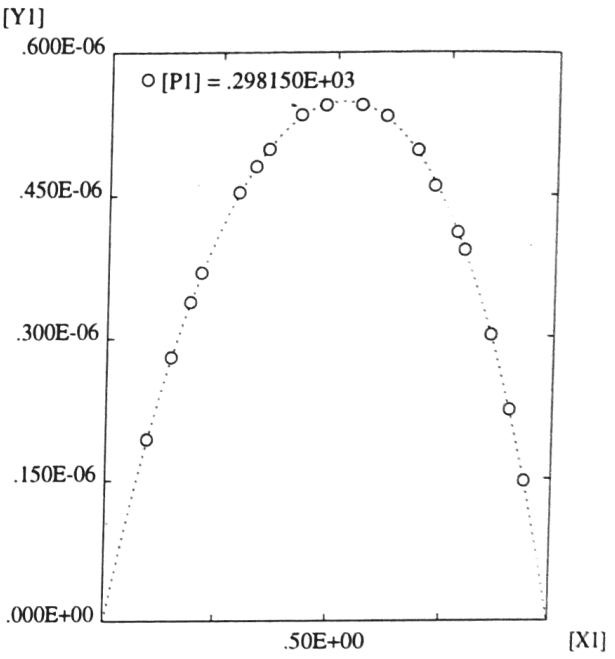

Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.008**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, Butan-2-ol**
2. $C_6H_{12}O_2$, Propyl propanoate

[P1] = .298150E+03

[X1]	[Y1]
.648000E–01	.117300E–06
.141000E+00	.250300E–06
.284800E+00	.406500E–06
.392300E+00	.467500E–06
.427900E+00	.476300E–06
.484900E+00	.486400E–06
.551000E+00	.481800E–06
.582900E+00	.477100E–06
.617500E+00	.464800E–06
.694300E+00	.423000E–06
.733300E+00	.390600E–06
.781400E+00	.345300E–06
.828600E+00	.293800E–06
.840100E+00	.275900E–06
.870100E+00	.231300E–06
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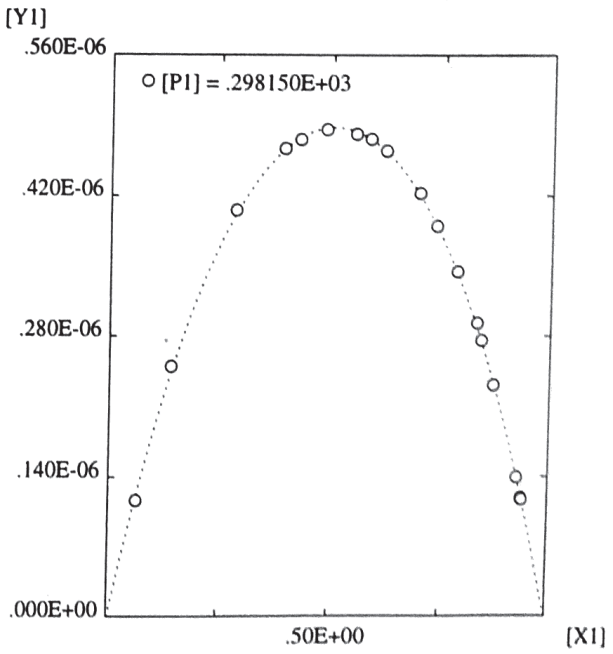

Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.009**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, Butan-2-ol**
2. $C_7H_{14}O_2$, Propyl butanoate

[P1] = .298150E+03

[X1]	[Y1]
.321000E-01	.633000E-07
.118900E+00	.221200E-06
.164200E+00	.280400E-06
.216500E+00	.346800E-06
.285900E+00	.406400E-06
.318700E+00	.432900E-06
.425700E+00	.473000E-06
.457700E+00	.479100E-06
.483900E+00	.486800E-06
.582800E+00	.474000E-06
.615000E+00	.460300E-06
.636700E+00	.451800E-06
.743500E+00	.368000E-06
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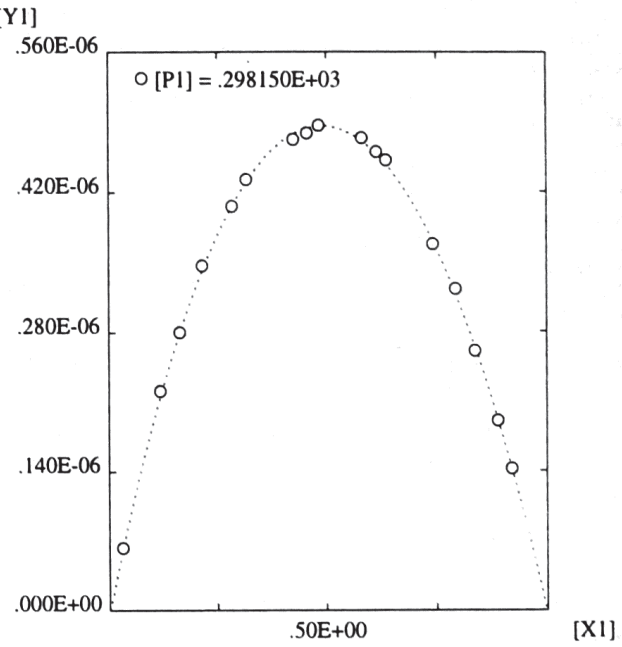


Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.010**

State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid

Parameters: [P1] T/K, Temperature

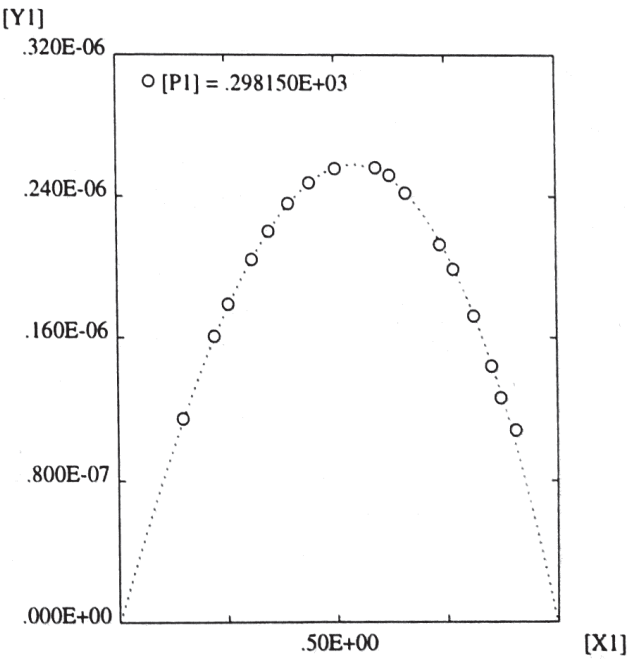
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume

Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, 2-Methylpropan-1-ol**
2. $C_5H_{10}O_2$, Propyl ethanoate

[P1] = .298150E+03

[X1]	[Y1]
.149300E+00	.115000E-06
.222400E+00	.160800E-06
.254800E+00	.178900E-06
.310600E+00	.204700E-06
.349200E+00	.220800E-06
.394100E+00	.236000E-06
.442600E+00	.247800E-06
.502100E+00	.255800E-06
.594100E+00	.256500E-06
.625700E+00	.252000E-06
.662400E+00	.242300E-06
.738200E+00	.213200E-06
.768400E+00	.199000E-06
.813400E+00	.172700E-06
.851800E+00	.144100E-06
.872400E+00	.126500E-06
.904800E+00	.108700E-06

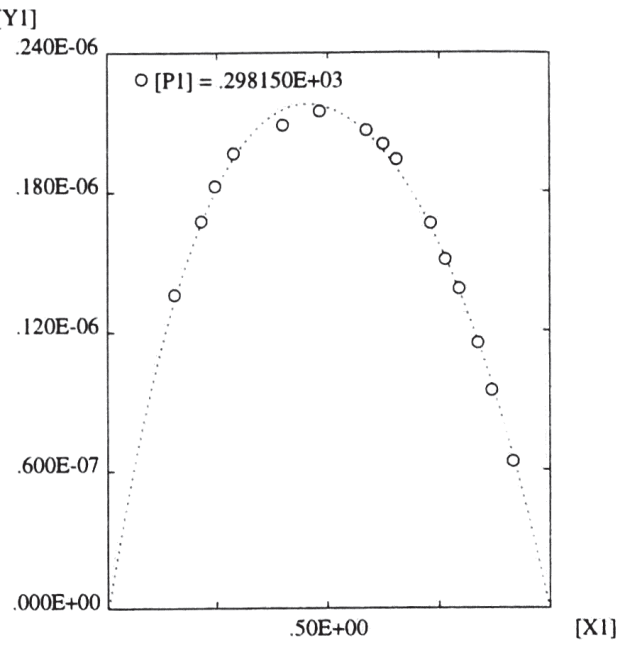


Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.011**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume
Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, 2-Methylpropan-1-ol**
2. $C_6H_{12}O_2$, Propyl propanoate

[P1] = .298150E+03

[X1]	[Y1]
.153500E+00	.136000E–06
.215000E+00	.167500E–06
.246700E+00	.182400E–06
.288800E+00	.196800E–06
.399800E+00	.208800E–06
.482600E+00	.215000E–06
.587100E+00	.206400E–06
.624000E+00	.200600E–06
.653900E+00	.193900E–06
.730100E+00	.166200E–06
.763200E+00	.150600E–06
.794800E+00	.138100E–06
.836700E+00	.114700E–06
.868000E+00	.944000E–07
.917100E+00	.637000E–07



Property Code: [VMSL1000] VOLUMETRIC PROPERTIES OF LIQUID MIXTURES AND SOLUTIONS **GONE0960.012**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] V^E/m^{3}mol^{-1}, Molar excess volume
Method: Calculation of V^E from low-pressure density measurements at variable x_1 and constant T

Components: **1. $C_4H_{10}O$, 2-Methylpropan-1-ol**
2. $C_7H_{14}O_2$, Propyl butanoate

[P1] = .298150E+03

[X1]	[Y1]
.179800E+00	.150800E–06
.221200E+00	.164800E–06
.325200E+00	.200600E–06
.385300E+00	.209700E–06
.523300E+00	.210300E–06
.556100E+00	.204000E–06
.605700E+00	.193000E–06
.676400E+00	.177900E–06
.680100E+00	.174900E–06
.777500E+00	.139900E–06
.828900E+00	.111500E–06
.840000E+00	.106000E–06
.898200E+00	.707000E–07
.944400E+00	.443000E–07