ORTJ0956

ELDATA: Int. Electron. J. Phys.-Chem. Data **1995**, *1*, 321-328

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

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Enthalpy-of-mixing measurements H^E are reported at 298.15 K for 12 binary 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 mixtures are endothermic.

1. INTRODUCTION

In continuation of our systematic experimental studies on the excess molar enthalpies H^E of mixtures containing alkanoates (esters) and alkanols (alcohols), [LOPM0860; ORTJ0954; SARF0880], we present here measurements at 298.15 K for 12 binary mixtures formed by four propyl n-alkanoates (methanoate, ethanoate, propanoate, and butanoate) with two alkan-2-ols (propan-2-ol and butan-2-ol) and an isoalkanol (2-methylpropan-1-ol). 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.

While many H^E data have been published in the literature for n-alkanoates + 1-alkanols, no data are found for the systems of this work.

2. EXPERIMENTAL SECTION

2.1. Apparatus and Procedure

The experimental data were taken at atmospheric pressure by means of a Calvet type microcalorimeter, model MS-80D (SETARAM, Lyon, France) with a stainless steel batch mixing cell (volume ca. 8 cm^3) and with negligible vapor phase described in [ORTJ0921]. The temperature T was maintained constant to within 0.02 K at (298.15 ± 0.02) K. All temperatures are on ITS-90. The microcalorimeter was calibrated electrically after each measurement (see [ORTJ0921]). Check measurements on cyclohexane + hexane and benzene + heptadecane are in agreement to within 1 % (over central range of concentration) with the data reported in [MCGM0690] and [DIAM0742]. The estimated uncertainties in the mole fraction composition x_i and H^E are, respectively, $\sigma(x_i) = 0.0005$ and $\sigma(H^E) = 0.02\ |H^E|$ (over central range of concentration).

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 %, 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 %, purified as above. n(D,298.15 K) = 1.3744; ρ(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 %, purified as above; 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 %, purified as above; 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 %. n(D,298.15 K) = 1.3820; ρ(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 %, purified as above; 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 %, purified as above; n(D, 298.15 K) = 1.3976; ρ_i(298.15 K)/kg m^{-3} = 868.07.

3. RESULTS

The direct experimental H^E values of the 12 systems are tabulated and graphed in the Appendix and saved on disk as Standard ELDATA Files **ORTJ0956.001** through **ORTJ0954.012**.

4. DISCUSSION AND CONCLUSIONS

All the mixtures are endothermic.

The data were fitted to Eq. (1):

$$H^E_{calc}/J\ mol^{-1} = x_1x_2\Sigma A_i[x_1/(x_1 + kx_2)]^{i-1} \quad (1)$$

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

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

where N is the number of experimental values, are less than 30 J mol^{-1} (less than 0.6 % at x_1 = 0.5).

For a given alkanol, the H^E decreases regularly with the increase of the chain-length of the alkanoate.

REFERENCES

[DIAM0742] – Diaz Pena, M.; Menduina, C. Excess enthalpies at 298.15 K of binary mixtures of benzene with n-alkanes. *J. Chem. Thermodyn.* **1974,** *6,* 387-393.

[LOPM0860] – Lopez, M.; Paz Andrade, M. I.; Fernandez, J.; Rodriguez-Nunez, E.; Ortega, J. Excess molar enthalpies at 298.15 K of (an n-alkyl formate + an n-alkanol). I. {xHCO2(CH2)3CH3 + (1-x)CnH2n+1OH}, (n = 3 to 10). *J. Chem. Thermodyn.* **1986,** *18,* 1003-1006.

[MCGM0690] – McGlashan, M. L.; Stoeckli, H. F. A flow calorimeter for enthalpies of mixing. The enthalpy of mixing of n-hexane + cyclohexane at 298.15 K. *J. Chem. Thermodyn.* **1969,** *1,* 589-594.

[ORTJ0954] – Ortega, J.; Chaar, M.; Placido, J. Excess enthalpies of 72 binary liquid mixtures of methyl n-alkanoates (C4 - C16) + alkan-1-ols (C2 - C10) at 298.15 K. *ELDATA Int. Electron. J. Phys.-Chem. Data* **1995,** *1,* 139-166.

[SARF0880] – Sarmiento, F.; Lopez, M.; Paz Andrade, M. I.; Fernandez, J.; Ortega, J.; Pena, J. A. Excess molar enthalpies at 298.15 K of (an n-alkyl formate + an n-alkanol). III. {xHCO2CH3 + (1-x)CnH2n+1OH}, (n = 3 to 10). *J. Chem. Thermodyn.* **1988,** *20,* 1315-1319.

Ortega, Juan* [ORTJ0]

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Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.001**

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] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E 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]
.675000E–01	.461200E+03
.139500E+00	.842100E+03
.210900E+00	.116110E+04
.279900E+00	.141040E+04
.342400E+00	.158400E+04
.409100E+00	.172490E+04
.457300E+00	.177880E+04
.503500E+00	.179750E+04
.544700E+00	.179520E+04
.586300E+00	.175270E+04
.634000E+00	.167690E+04
.684100E+00	.156570E+04
.737800E+00	.140760E+04
.792900E+00	.120470E+04
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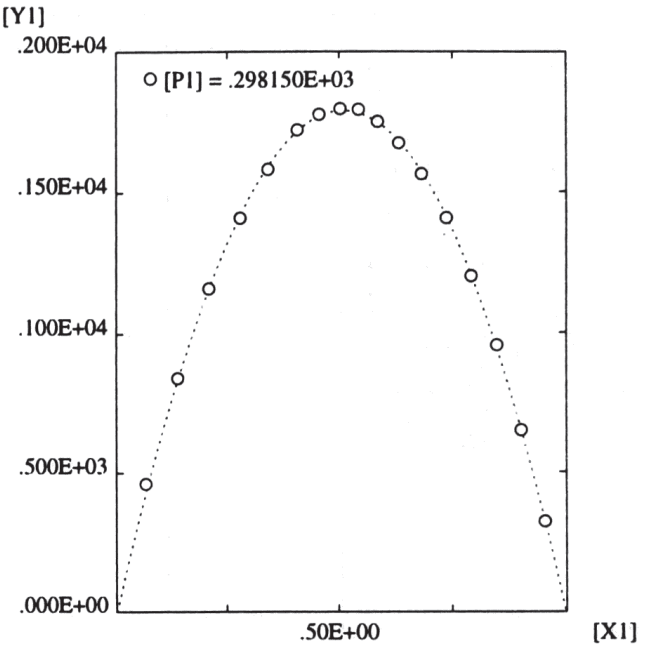

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.002**

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] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E 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]
.826000E–01	.539400E+03
.168300E+00	.933900E+03
.250900E+00	.126780E+04
.328900E+00	.149880E+04
.399800E+00	.164480E+04
.433200E+00	.169430E+04
.494500E+00	.172770E+04
.549100E+00	.172490E+04
.596700E+00	.167560E+04
.675600E+00	.154430E+04
.722600E+00	.141620E+04
.771600E+00	.125200E+04
.820900E+00	.105150E+04
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.917200E+00	.552900E+03
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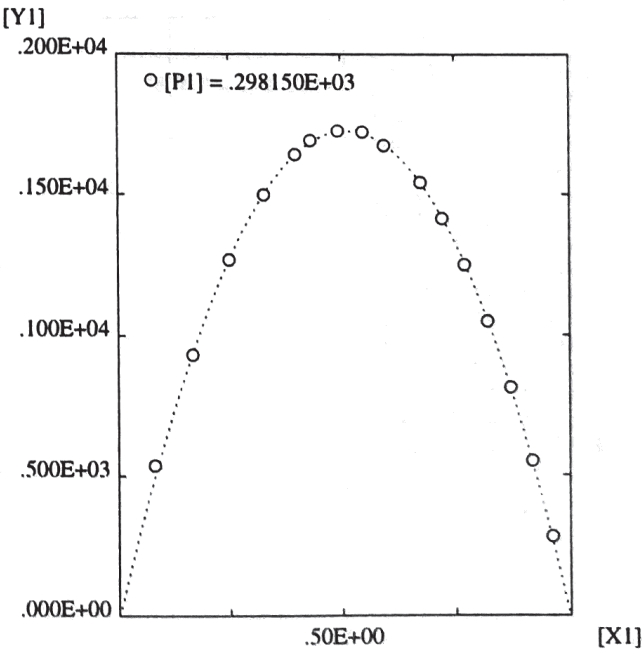

ORTJ0956.003

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.101400E+00	.624700E+03
.195500E+00	.106250E+04
.284400E+00	.137640E+04
.367200E+00	.156700E+04
.441300E+00	.166620E+04
.506200E+00	.168180E+04
.562100E+00	.166730E+04
.617800E+00	.159590E+04
.659100E+00	.151750E+04
.702000E+00	.142390E+04
.746700E+00	.129180E+04
.792200E+00	.113110E+04
.838700E+00	.928200E+03
.883400E+00	.725100E+03
.925600E+00	.503700E+03
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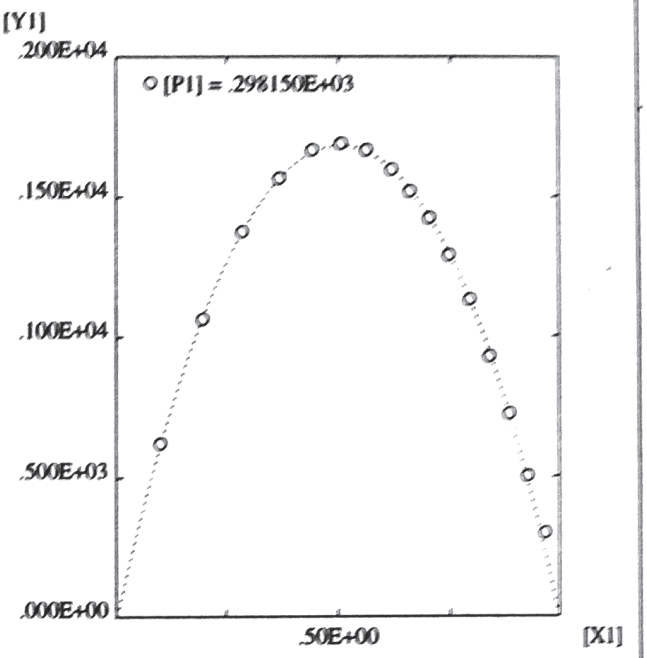

ORTJ0956.004

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.101100E+00	.638700E+03
.206500E+00	.109780E+04
.304100E+00	.140360E+04
.392200E+00	.158230E+04
.468300E+00	.164880E+04
.532600E+00	.164480E+04
.587800E+00	.160080E+04
.635200E+00	.153080E+04
.675400E+00	.144610E+04
.710200E+00	.135640E+04
.773100E+00	.113810E+04
.816800E+00	.970000E+03
.858700E+00	.793600E+03
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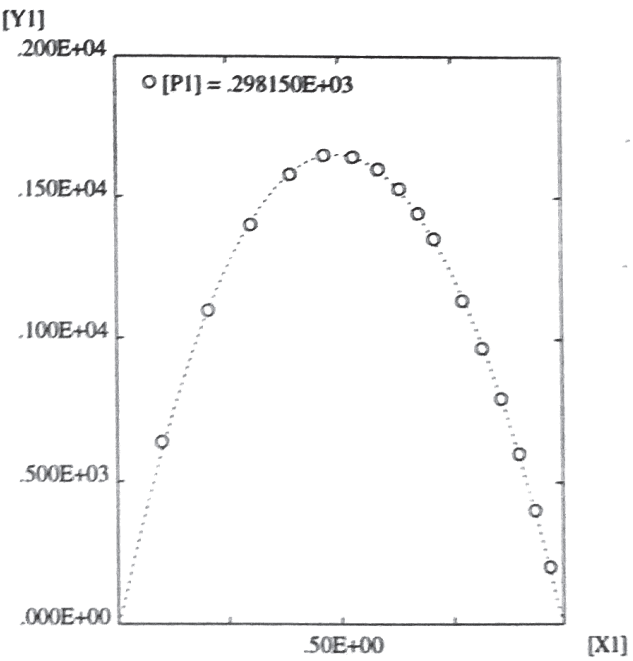
.969800E+00	.202900E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.005**

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

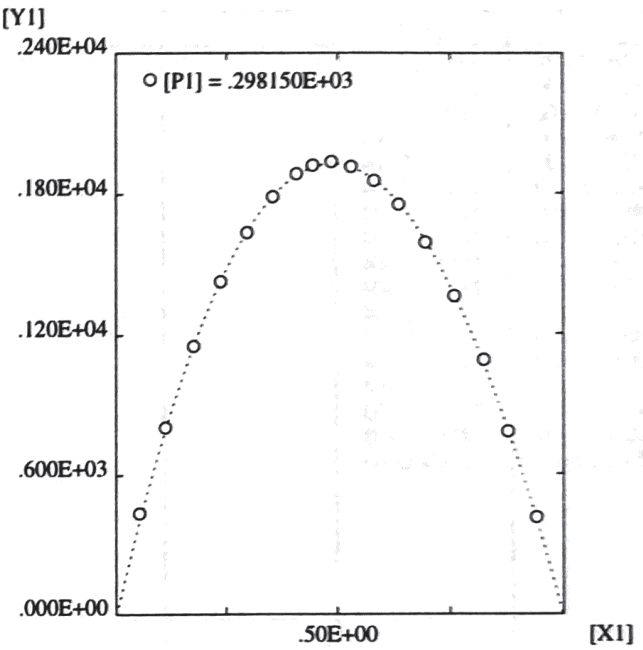
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E 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]
.540000E-01	.435500E+03
.113800E+00	.806900E+03
.176600E+00	.115420E+04
.238100E+00	.142870E+04
.297800E+00	.163730E+04
.355500E+00	.178940E+04
.409200E+00	.188580E+04
.445000E+00	.192000E+04
.486100E+00	.193650E+04
.530900E+00	.191660E+04
.581800E+00	.185540E+04
.637100E+00	.175250E+04
.696200E+00	.159220E+04
.759600E+00	.136490E+04
.825400E+00	.108940E+04
.878500E+00	.783900E+03
.941500E+00	.416500E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.006**

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

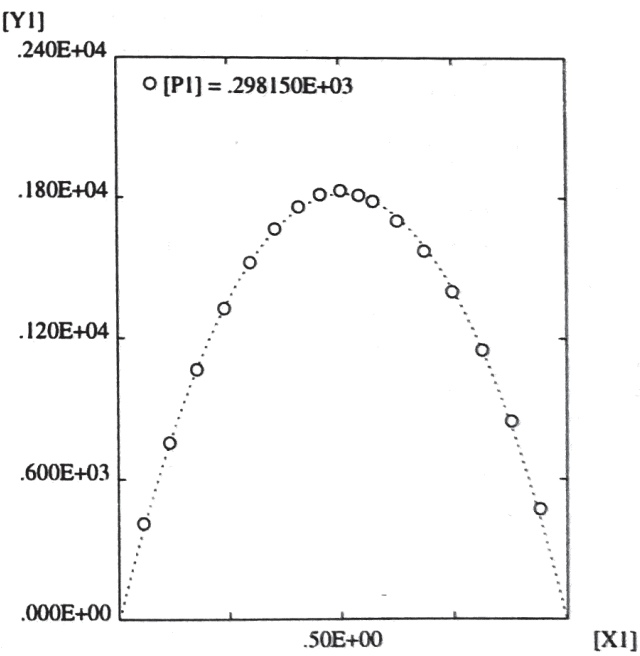
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E 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]
.571000E-01	.412300E+03
.117100E+00	.756100E+03
.178300E+00	.106840E+04
.240800E+00	.132600E+04
.300900E+00	.152430E+04
.357800E+00	.166830E+04
.410600E+00	.176370E+04
.458900E+00	.181760E+04
.503500E+00	.183360E+04
.544000E+00	.181260E+04
.575400E+00	.178920E+04
.629400E+00	.170400E+04
.687700E+00	.157680E+04
.749700E+00	.140190E+04
.814100E+00	.115430E+04
.878600E+00	.849200E+03
.941200E+00	.471500E+03



ORTJ0956.007

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.786000E-01	.536100E+03
.156900E+00	.942300E+03
.232100E+00	.130080E+04
.309400E+00	.157170E+04
.377100E+00	.174350E+04
.440200E+00	.184220E+04
.496200E+00	.187890E+04
.505200E+00	.188290E+04
.545800E+00	.185460E+04
.589800E+00	.181230E+04
.636900E+00	.173330E+04
.686000E+00	.162480E+04
.739600E+00	.145430E+04
.793700E+00	.124120E+04
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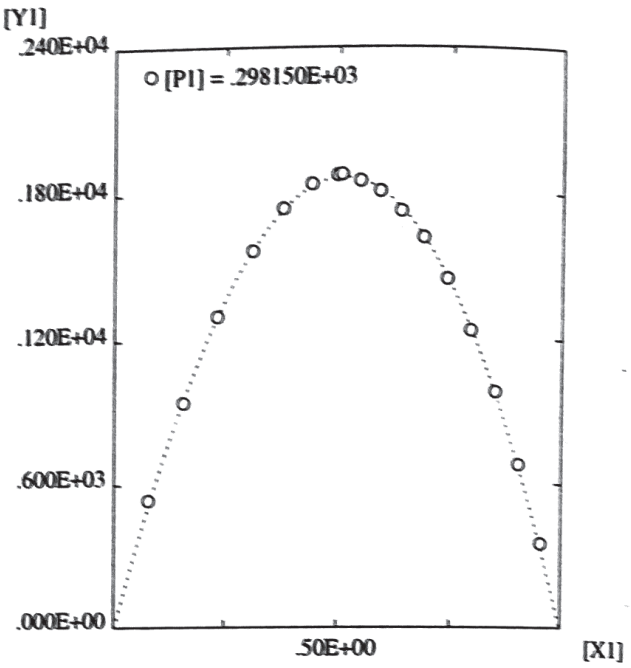

ORTJ0956.008

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.791000E-01	.548100E+03
.158500E+00	.968400E+03
.237200E+00	.131570E+04
.310600E+00	.155950E+04
.379800E+00	.171760E+04
.442800E+00	.179920E+04
.498700E+00	.182540E+04
.535800E+00	.181690E+04
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.765300E+00	.131080E+04
.814900E+00	.110220E+04
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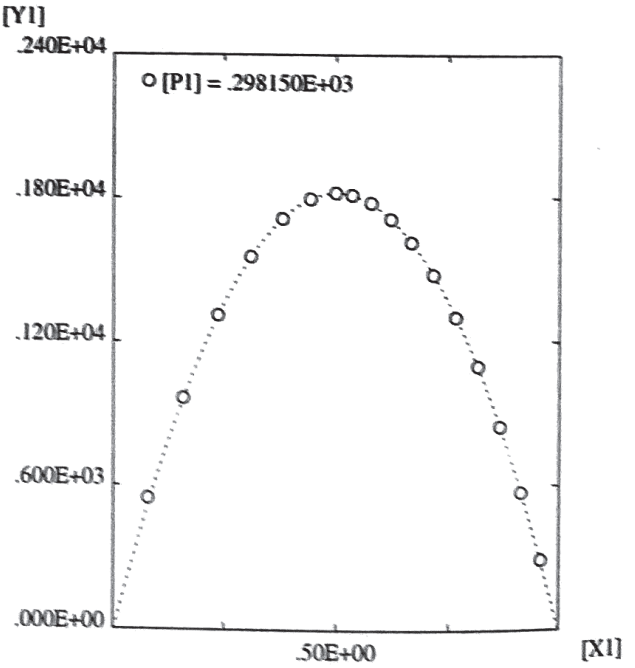

ORTJ0956.009

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.860000E-01	.593900E+03
.177400E+00	.105130E+04
.263300E+00	.139860E+04
.343100E+00	.161990E+04
.415400E+00	.174430E+04
.480100E+00	.179290E+04
.536000E+00	.178730E+04
.585100E+00	.174810E+04
.628500E+00	.167450E+04
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.814700E+00	.107260E+04
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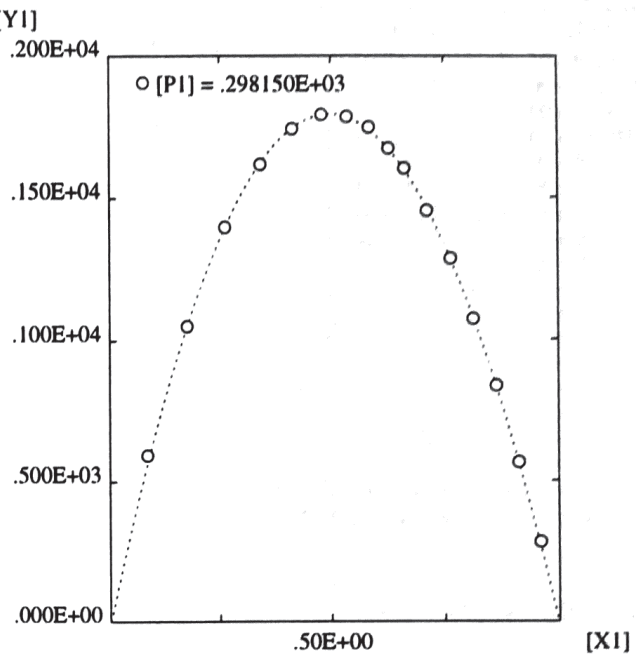


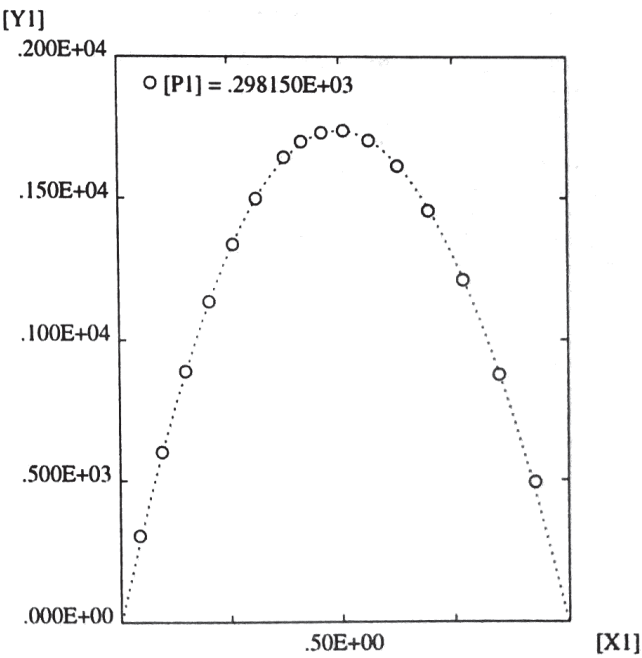
ORTJ0956.010

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.450000E-01	.309100E+03
.958000E-01	.603500E+03
.150500E+00	.891600E+03
.205200E+00	.113670E+04
.260100E+00	.133970E+04
.313100E+00	.149760E+04
.376900E+00	.164670E+04
.416500E+00	.170200E+04
.461000E+00	.173490E+04
.510400E+00	.174120E+04
.566800E+00	.170590E+04
.629100E+00	.161600E+04
.696000E+00	.145950E+04
.770800E+00	.121300E+04
.848900E+00	.877500E+03
.927100E+00	.494200E+03

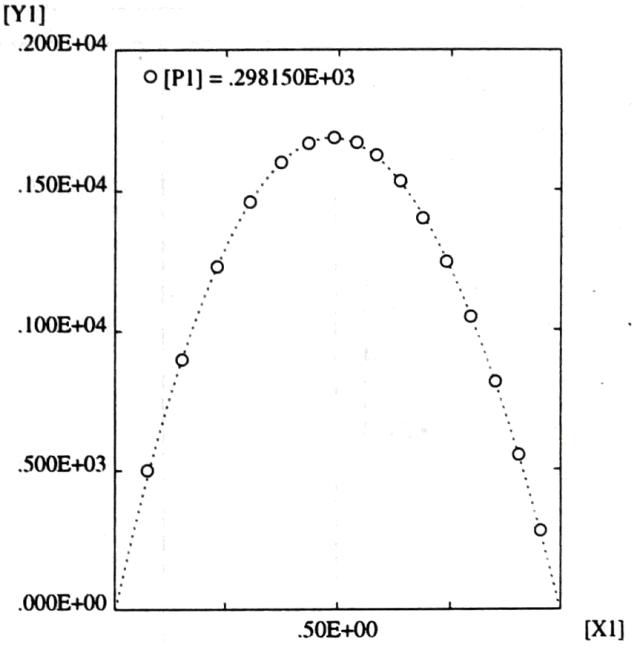


Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.011**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.736000E–01	.501500E+03
.151700E+00	.899800E+03
.230100E+00	.123080E+04
.304600E+00	.146170E+04
.372400E+00	.160090E+04
.433700E+00	.166970E+04
.489700E+00	.168920E+04
.539300E+00	.167020E+04
.583400E+00	.162660E+04
.636800E+00	.153480E+04
.686500E+00	.140020E+04
.740000E+00	.124510E+04
.795000E+00	.104960E+04
.850200E+00	.815400E+03
.904000E+00	.554400E+03
.954600E+00	.281500E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0956.012**
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] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E 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]
.944000E–01	.618500E+03
.187100E+00	.104610E+04
.279500E+00	.136990E+04
.362500E+00	.156360E+04
.435000E+00	.165090E+04
.498800E+00	.166980E+04
.555400E+00	.164390E+04
.598700E+00	.157040E+04
.641600E+00	.149920E+04
.686800E+00	.138950E+04
.733400E+00	.125390E+04
.779600E+00	.110040E+04
.828000E+00	.912100E+03
.876600E+00	.693700E+03
.922700E+00	.455200E+03
.964400E+00	.222600E+03