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Excess enthalpies of 14 binary liquid mixtures of .alpha.,.omega.-dihalo (Cl, Br, I)alkanes (C2-C6) + cyclohexane. Experimental data and group contribution (DISQUAC) analysis of an extended database

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Enthalpy-of-mixing H^E measurements are reported at 298.15 K for 14 binary liquid mixtures containing 1,ω-dihalo(Cl, Br, I)alkanes (ω = 2,3,4,5,6) + cyclohexane over the entire range of composition. These experimental results, along with our previous H^E data for the mixtures formed by the same 1,ω-dihaloalkanes with n-alkanes, a database of 96 binary systems, are interpreted in terms of the DISQUAC group-contribution model. Revised quasi-chemical parameters are presented. The predicted H^E data are in agreement with experiment to within 5 to 7 %.

1. INTRODUCTION

The literature contains several studies on binary mixtures of various halogenated alkanes with aliphatic (linear or cyclic) or aromatic hydrocarbons as a test of the applicability of the DISQUAC and other group-contribution models to predict the thermodynamic properties of this class of systems [ARTM0914; KEHH0880; MUNJ0871; PLAJ0951; SORM0891].

In order to know more exactly the behavior of mixtures containing dihaloalkanes, we have first measured the molar excess enthalpies H^E of 82 binary liquid mixtures containing α,ω-dihalo(Cl, Br, I)alkanes (C_2 - C_6) + n-alkanes (C_5 - C_{17}) [ORTJ0930; ORTJ0932; ORTJ0933], critically reviewed all the literature data, and then analyzed the entire database using several versions of the UNIFAC model [ORTJ0957]).

The purpose of the present paper is to report additional H^E measurements for 14 binary liquid mixtures containing α,ω-dihalo(Cl, Br, I)alkanes (C_2 - C_6) + cyclohexane over the entire range of composition. These experimental results, along with our previous H^E data for the mixtures formed by the same α,ω-dihaloalkanes with n-alkanes, i. e. a database of 96 binary systems, are now interpreted in terms of the DISQUAC model [KEHH0830; KEHH0850].

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 [ORTJ0921]. The temperature T (ITS-90) was maintained constant at (298.15 ± 0.02) K. The microcalorimeter was calibrated electrically after each measurement. 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

$C_2H_4Br_2$, 1,2-Dibromoethane (Ethylene dibromide). Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D, 298.15 K) = 1.5356 (1.5360 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 2168.26 (2168.7 [RIDJ0860]).

$C_2H_4Cl_2$, 1,2-Dichloroethane (Ethylene dichloride). Fluka AG (Buchs, Switzerland) 'puriss' grade material of stated GLC purity > 99.5 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.4422 (1.4421 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 1245.38 (1246.37 [RIDJ0860]).

$C_3H_6Br_2$, 1,3-Dibromopropane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.5204 (1.5208 [TRC00640]); ρ(298.15 K)/kg m^{-3} = 1970.14 (1971.3 [TRC00640]).

$C_3H_6Cl_2$, 1,3-Dichloropropane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 %, was purified as above and used without further

TABLE 1

New quasi-chemical DISQUAC interchange energy coefficients, $C_{ad,i}^{quac} = C_{bd,i}^{quac}$, for different classes of α,ω-dihaloalkanes, XCH_2-$(CH_2)_{u-2}$-CH_2X (X = Cl, Br, I) with n-alkanes or cyclohexane for contacts (a,d) and (b,d), a = CH_2 in n-alkanes, b = CH_2 in cyclohexane, d = X (this work)

	$u = 2$	$u = 3$	$u = 4$	$u > 4$
$i = 1$ (*Gibbs energy coefficient*)				
X = I	1.42	1.66	1.85	1.98
$i = 2$ (*enthalpy coefficient*)				
X = Cl	3.23	3.67	4.03	4.14
X = Br	2.51	3.07	3.49	3.80
X = I	2.00	2.69	3.14	3.34

purification. n(D, 298.15 K) = 1.4455 (1.4460 [TRC00640]; ρ(298.15 K)/kg m^{-3} = 1178.45 (1181.8 [TRC00640]).

$C_3H_6I_2$, 1,3-Diiodopropane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 mole %, was purified as above and used without further purification. n(D, 298.15 K) = 1.6391; ρ(298.15 K)/kg m^{-3} = 2561.21.

$C_4H_8Br_2$, 1,4-Dibromobutane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.5167 (1.5169 [TRC00640]); ρ(298.15 K)/kg m^{-3} = 1819.90 (1818.7 [TRC00640]).

$C_4H_8Cl_2$, 1,4-Dichlorobutane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.4522 (1.4522 [TRC00640]; ρ(298.15 K)/kg m^{-3} = 1133.06 (1135.3 [TRC00640]).

$C_4H_8I_2$, 1,4-Diiodobutane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.6184; ρ(298.15 K)/kg m^{-3} = 2349.38.

$C_5H_{10}Br_2$, 1,5-Dibromopentane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 97 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.5102 (1.5103 [TRC00640]); ρ(298.15 K)/kg m^{-3} = 1692.80 (1694.8 [TRC00640]).

$C_5H_{10}Cl_2$, 1,5-Dichloropentane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 99 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.4545 (1.4541 [TRC00640]; ρ(298.15 K)/kg m^{-3} = 1095.60 (1095.6 [TRC00640]).

$C_5H_{10}I_2$, 1,5-Diiodopentane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 97 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.5987; ρ(298.15 K)/kg m^{-3} = 2169.16.

C_6H_{12}, Cyclohexane. Fluka AG (Buchs, Switzerland) 'puriss' grade material of stated GLC purity > 99.5 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.4235 (1.42354 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 773.85 (773.89 [RIDJ0860]).

$C_6H_{12}Br_2$, 1,6-Dibromohexane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 96 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.5054; ρ(298.15 K)/kg m^{-3} = 1602.49.

$C_6H_{12}Cl_2$, 1,6-Dichlorohexane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 98 %, was purified as above and used without further purification. n(D, 298.15 K) = 1.4555; ρ(298.15 K)/kg m^{-3} = 1067.59.

$C_6H_{12}I_2$, 1,6-Diiodohexane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity 97 %, purified as above and used without further purification. n(D, 298.15 K) = 1.5837; ρ(298.15 K)/kg m^{-3} = 2034.19.

3. RESULTS

The direct experimental H^E values are tabulated and graphed in the Appendix and saved on disk as Standard ELDATA Files **PLAJ0970.001** through **PLAJ0970.014**.

The data were fitted to Eq. (1):

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

all points weighted equally. With an adjusted coefficient k and n = 2 coefficients A_i, the standard deviations

$\sigma(H^E)$, defined by Eq.(2):

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

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

For 1,2-dichloroethane + cyclohexane our results agree fairly well (within 3 %, at $x_1 = 0.5$) with the values reported by [BANI0830; KORA3690]; VIGJ0810] , but differ from those of [TSCH0484; AMAK0580; MAHB0771]. For 1,3-dichloropropane + cyclohexane our results differ by as much as 200 J mol^{-1} (at $x_1 = 0.5$) from those of [BANI0900]. The data reported by [ARTM0914] for α,ω-dibromoalkanes + cyclohexane differ from our measurements by 170 J mol^{-1} (at x_1 = 0.5) for 1,3-dibromopropane, the differences decreasing progressively with the chain-length of the dibromoalkane, being 71 J mol^{-1} for 1,6-dibromohexane. For 1,2-dibromoethane + cyclohexane our results agree (within 4%, at $x_1 = 0.5$) with the values reported by [PERP0830; KALK0900], but differ from those of [MAHB0760].

4. APPLICATION OF THE DISQUAC MODEL

4.1. Comparison using the old interaction parameters

The DISQUAC equations used to calculate H^E, the geometrical description of the molecules, and the geometrical parameters were the same as published before by [ARTM0914; KEHH0880; MUNJ0871; PLAJ0951; SORM0891]. At the beginning, we have compared the experimental data of our extended database with those predicted using the previously published interaction parameters.

The parameters reported by [KEHH0880] for α,ω-dichloroalkanes + n-alkanes or + cyclohexane gave an overall mean difference of 9.5 % with n-alkanes and 11 % with cyclohexane.

For α,ω-dibromoalkanes + n-alkanes or + cyclohexane we used the parameters reported by [ARTM0914] and the overall mean difference was less than 12 %.

No interaction parameters have been reported for α,ω-diiodoalkanes + n-alkanes or + cyclohexane. Using the parameters of 1-iodoalkanes [MUNJ0871; SORM0891], the overall mean differences for 1,5-diiodopentane and 1,6-diiodohexane, the only miscible α,ω-diiodoalkanes, were 15 % for n-alkanes and 21 % for cyclohexane.

The excess enthalpies of α,ω-dichloroalkanes or α,ω-dibromoalkanes + n-alkanes (a) or + cyclohexane (b) predicted with the old parameters of the DISQUAC model are acceptable. Nevertheless, we decided to recalculate the enthalpic quasi-chemical parameters, $C^{quac}_{ad,2} = C^{quac}_{bd,2}$, for the Cl/$CH_2$ and Br/CH_2 contacts using our extended database and to estimate all the interaction parameters of the I/CH_2 contact in α,ω-diiodoroalkanes, accounting also for the proximity effect.

4.2. Estimation of new interaction parameters

The dispersive interaction parameters $C^{dis}_{ad,i} = C^{dis}_{bd,i}$ were the same as before, except $C^{dis}_{bd,2} = 0.45$ for α,ω-diiodoalkanes + cyclohexane which has been adjusted according to the new data.

The $C^{quac}_{ad,2} = C^{quac}_{bd,2}$ parameters depend on the distance u between the halogen atoms X in the α,ω-dihaloalkane, XCH_2-$(CH_2)_{u-2}CH_2X$ ('proximity effect'). These were recalculated separately, by regression, for each type of mixtures and are listed in Table 1. Included are also guessed Gibbs energy parameters, $C^{quac}_{ad,1}$, for the I/CH_2 contact in α,ω-diiodoroalkanes.

The new parameters differ but only slightly from the previous ones. The calculated H^E values at 298.15 K agree now to within 5 % in the average with the experimental data of the 82 α,ω-dihaloalkane + n-alkane mixtures and within 7 % in the average with the experimental data of the 14 α,ω-dihaloalkane + cyclohexane mixtures. For the partially miscible 1,4-diiodobutane (1) + heptane (2) system, at $x_1 = 0.228$ (totally miscible) the calculated H^E = 1346 J mol^{-1} reproduces correctly the experimental value of 1340 J mol^{-1} (unpublished data from this Laboratory).

5. DISCUSSION AND CONCLUSIONS

As expected, the excess enthalpies of α,ω-dihaloalkane + cyclohexane mixtures are all positive, slightly lower than in mixtures with hexane, and decrease with increasing the chain-length of the α,ω-dihaloalkane. DISQUAC appears to be reliable predictive method.

The readjustment of the enthalpic quasi-chemical parameters improved the overall agreement with experiment. The present study also confirmed the existence of the proximity effect in α,ω-diiodoalkanes. As in the case of Cl or Br, the corresponding interaction parameters increase with the distance u between the I atoms reaching the values of 1-iodoalkanes when $u > 4$. Accurate vapor-liquid equilibrium data are however needed in order to optimize the I/CH_2 Gibbs energy interaction parameters.

The Modified UNIFAC [GMEJ0930] predictions of the excess enthalpies of the same α,ω-dihaloalkane + cyclohexane mixtures agree with the experimental data within 15 % in the average. Using the UNIFAC parameters we proposed previously [ORTJ0957], the agreement is close to 6 %.

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Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.006**
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. $C_2H_4Br_2$, 1,2-Dibromoethane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.740000E-01	.458100E+03
.145400E+00	.762400E+03
.222300E+00	.102100E+04
.292200E+00	.118970E+04
.358700E+00	.130090E+04
.421300E+00	.137490E+04
.478400E+00	.139850E+04
.528800E+00	.141020E+04
.573300E+00	.138180E+04
.645700E+00	.128600E+04
.695500E+00	.118930E+04
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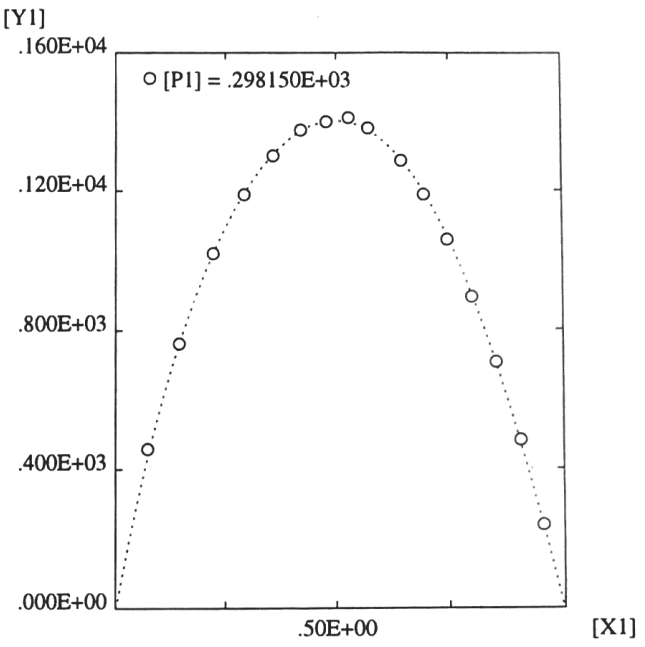

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.001**
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Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_2H_4Cl_2$, 1,2-Dichloroethane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.742000E-01	.357200E+03
.153600E+00	.722100E+03
.234800E+00	.105500E+04
.309200E+00	.128750E+04
.379400E+00	.143580E+04
.442800E+00	.151590E+04
.499800E+00	.154590E+04
.515800E+00	.154830E+04
.556900E+00	.153270E+04
.600900E+00	.149230E+04
.647700E+00	.142580E+04
.698300E+00	.132270E+04
.749700E+00	.118180E+04
.802400E+00	.100470E+04
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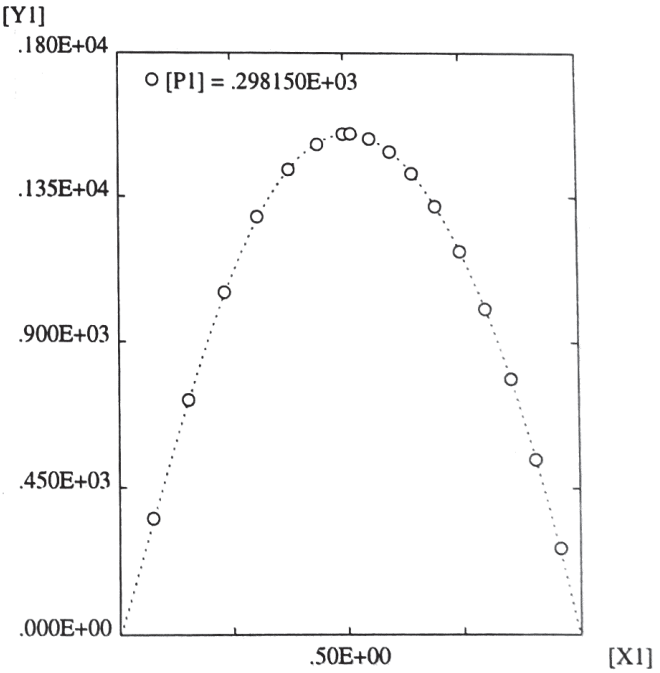
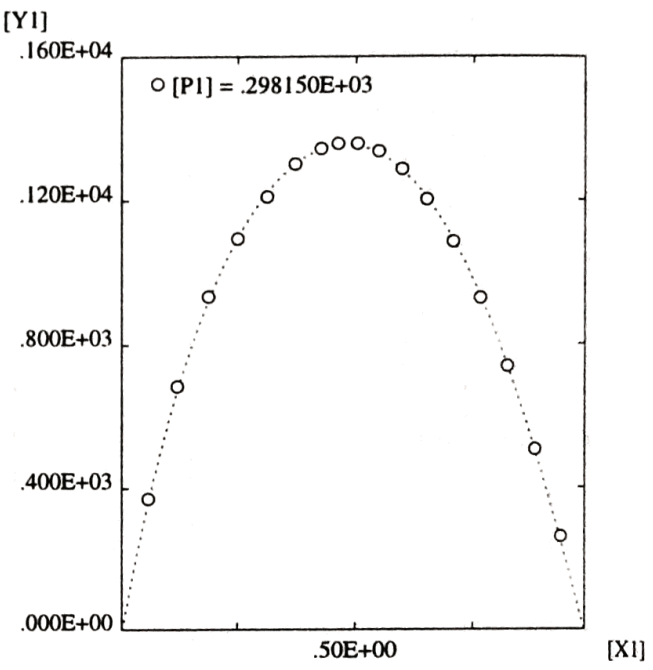


Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.007**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_3H_6Br_2$, 1,3-Dibromopropane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.583000E–01	.371600E+03
.121400E+00	.684400E+03
.187500E+00	.935900E+03
.251300E+00	.109440E+04
.313800E+00	.121050E+04
.372100E+00	.130380E+04
.426800E+00	.134490E+04
.463300E+00	.135960E+04
.504000E+00	.135950E+04
.549100E+00	.133740E+04
.597300E+00	.128770E+04
.651100E+00	.120370E+04
.707300E+00	.108510E+04
.766000E+00	.928300E+03
.825200E+00	.738200E+03
.886800E+00	.506900E+03
.946800E+00	.263600E+03

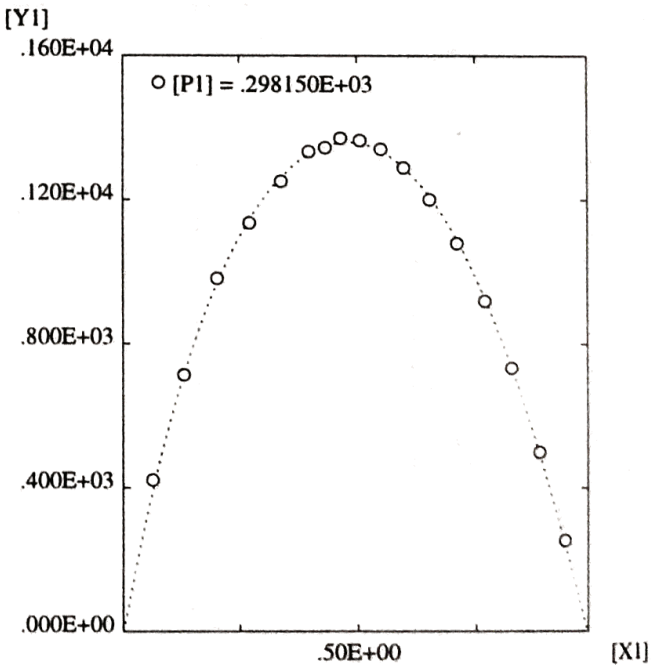


Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.002**
State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
Pure component 1, liquid
Pure component 2, liquid
Parameters: [P1] T/K, Temperature
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy
Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_3H_6Cl_2$, 1,3-Dichloropropane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.644000E–01	.423100E+03
.132600E+00	.715100E+03
.203700E+00	.982300E+03
.273300E+00	.113650E+04
.339800E+00	.125310E+04
.399900E+00	.133520E+04
.433900E+00	.134790E+04
.466100E+00	.137210E+04
.507000E+00	.136620E+04
.550500E+00	.134200E+04
.599700E+00	.129120E+04
.654500E+00	.120350E+04
.711400E+00	.108050E+04
.770500E+00	.920300E+03
.829600E+00	.734700E+03
.890500E+00	.501800E+03
.947600E+00	.254900E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.011**

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

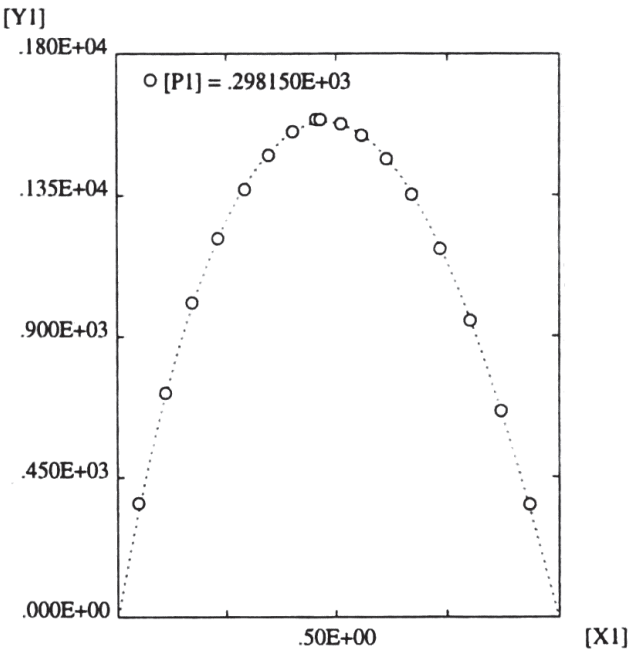
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_3H_6I_2$, 1,3-Diiodopropane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.493000E-01	.368500E+03
.111800E+00	.720400E+03
.172700E+00	.100860E+04
.232100E+00	.121460E+04
.293000E+00	.137000E+04
.347600E+00	.147610E+04
.401600E+00	.155060E+04
.454700E+00	.159050E+04
.465500E+00	.158860E+04
.511100E+00	.157720E+04
.559300E+00	.154110E+04
.614500E+00	.146510E+04
.671300E+00	.135310E+04
.735600E+00	.118110E+04
.802400E+00	.950500E+03
.871000E+00	.661900E+03
.935800E+00	.363000E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.008**

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

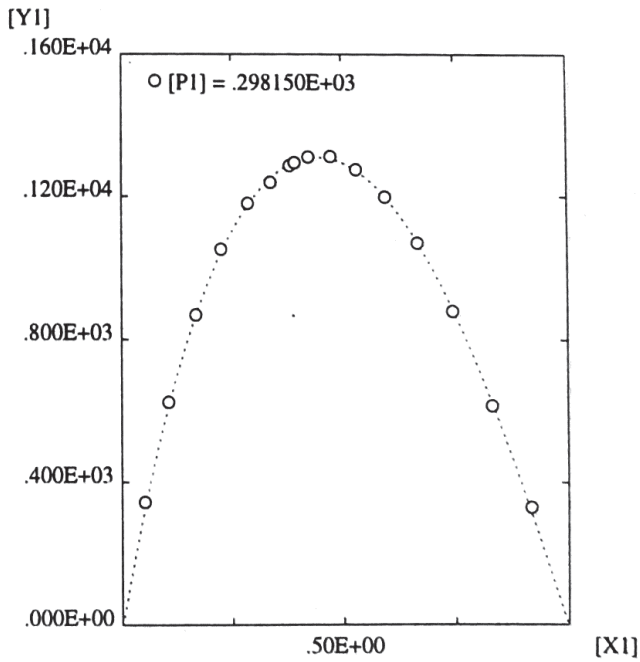
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_4H_8Br_2$, 1,4-Dibromobutane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.524000E-01	.344800E+03
.107200E+00	.625800E+03
.169300E+00	.869300E+03
.227800E+00	.105230E+04
.288500E+00	.118080E+04
.340300E+00	.123930E+04
.383200E+00	.128660E+04
.395100E+00	.129560E+04
.426500E+00	.131160E+04
.476400E+00	.131280E+04
.534200E+00	.127590E+04
.597000E+00	.119990E+04
.668800E+00	.107060E+04
.746200E+00	.881200E+03
.832100E+00	.617700E+03
.917900E+00	.331900E+03



PLAJ0970.003

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. $C_4H_8Cl_2$, 1,4-Dichlorobutane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.530000E–01	.355000E+03
.111300E+00	.613100E+03
.174800E+00	.843100E+03
.237100E+00	.100930E+04
.299100E+00	.112730E+04
.357100E+00	.119950E+04
.411600E+00	.124110E+04
.460600E+00	.125820E+04
.506600E+00	.125100E+04
.548300E+00	.123820E+04
.570000E+00	.122450E+04
.626600E+00	.114980E+04
.687300E+00	.103730E+04
.752300E+00	.882700E+03
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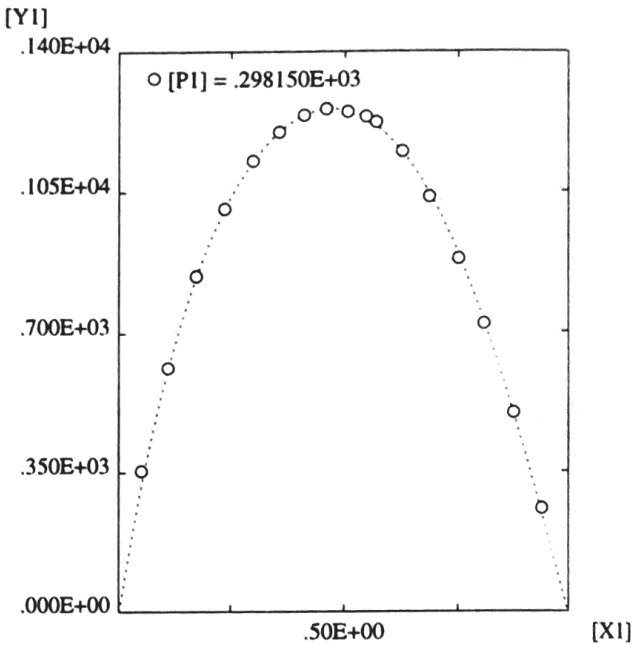
.876300E+00	.497500E+03
.940000E+00	.258500E+03



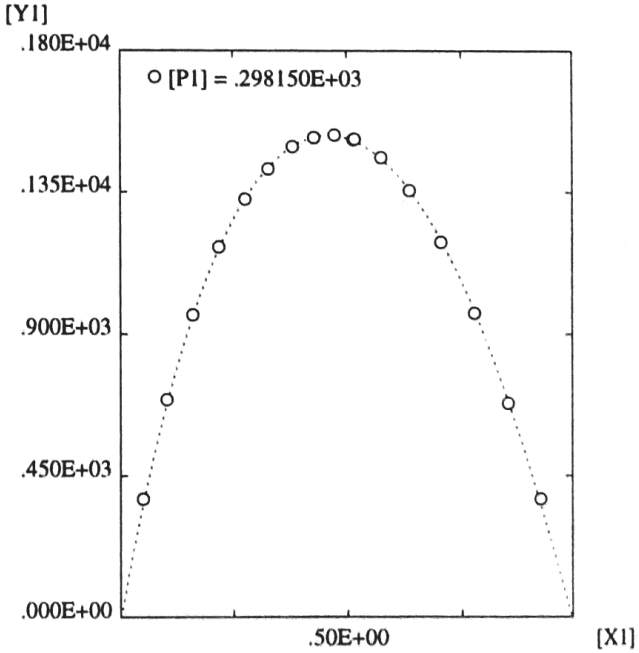
PLAJ0970.012

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. $C_4H_8I_2$, 1,4-Diiodobutane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.502000E–01	.376900E+03
.104200E+00	.694000E+03
.161000E+00	.961100E+03
.219200E+00	.117780E+04
.276600E+00	.132940E+04
.329400E+00	.142590E+04
.381900E+00	.149470E+04
.429200E+00	.152480E+04
.474300E+00	.153260E+04
.514800E+00	.151750E+04
.518100E+00	.152000E+04
.575300E+00	.146060E+04
.636500E+00	.135870E+04
.705900E+00	.119390E+04
.778200E+00	.969000E+03
.853500E+00	.683200E+03
.927700E+00	.376400E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.009**

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

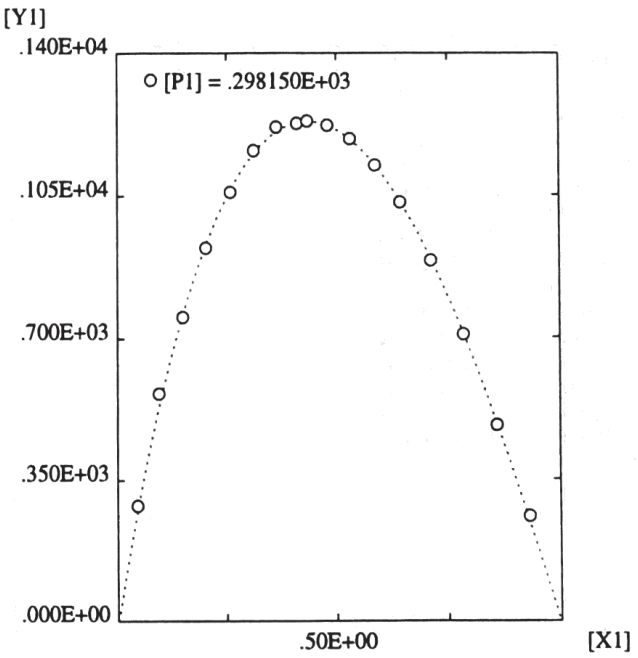
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_5H_{10}Br_2$, 1,5-Dibromopentane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.456000E–01	.288400E+03
.962000E–01	.564200E+03
.150500E+00	.753400E+03
.204500E+00	.923100E+03
.260100E+00	.106030E+04
.314000E+00	.116120E+04
.364900E+00	.121820E+04
.411500E+00	.122730E+04
.434700E+00	.123230E+04
.480700E+00	.122280E+04
.531300E+00	.118940E+04
.588800E+00	.112350E+04
.645000E+00	.103290E+04
.713300E+00	.890200E+03
.784700E+00	.707900E+03
.860300E+00	.484400E+03
.931600E+00	.259300E+03



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **PLAJ0970.004**

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

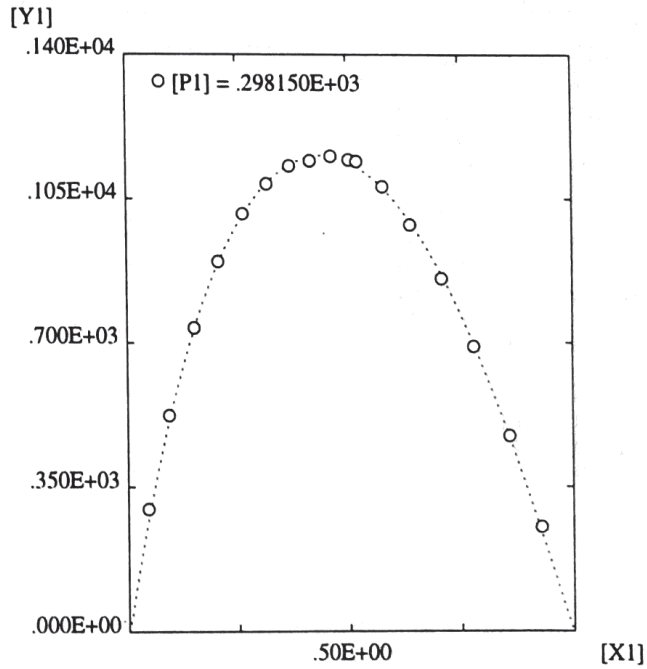
Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] H^E/J mol^{-1}, Molar excess enthalpy

Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: **1. $C_5H_{10}Cl_2$, 1,5-Dichloropentane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.468000E–01	.297400E+03
.952000E–01	.524600E+03
.152300E+00	.737000E+03
.209100E+00	.899100E+03
.265400E+00	.101400E+04
.318800E+00	.108820E+04
.370900E+00	.113120E+04
.418500E+00	.114380E+04
.464100E+00	.115330E+04
.505200E+00	.114580E+04
.523100E+00	.114150E+04
.579900E+00	.108090E+04
.642100E+00	.988600E+03
.709700E+00	.857100E+03
.780900E+00	.692200E+03
.857900E+00	.475800E+03
.929000E+00	.253000E+03



PLAJ0970.013

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. $C_5H_{10}I_2$, 1,5-Diiodopentane**
2. C_6H_{12} , Cyclohexane

[P1] = .298150E+03

[X1]	[Y1]
.400000E–01	.293400E+03
.933900E–01	.607400E+03
.154600E+00	.901900E+03
.213300E+00	.108490E+04
.270800E+00	.123580E+04
.322600E+00	.132660E+04
.370600E+00	.138500E+04
.408500E+00	.142360E+04
.453200E+00	.142590E+04
.502500E+00	.140770E+04
.559500E+00	.135390E+04
.622300E+00	.125480E+04
.691200E+00	.110460E+04
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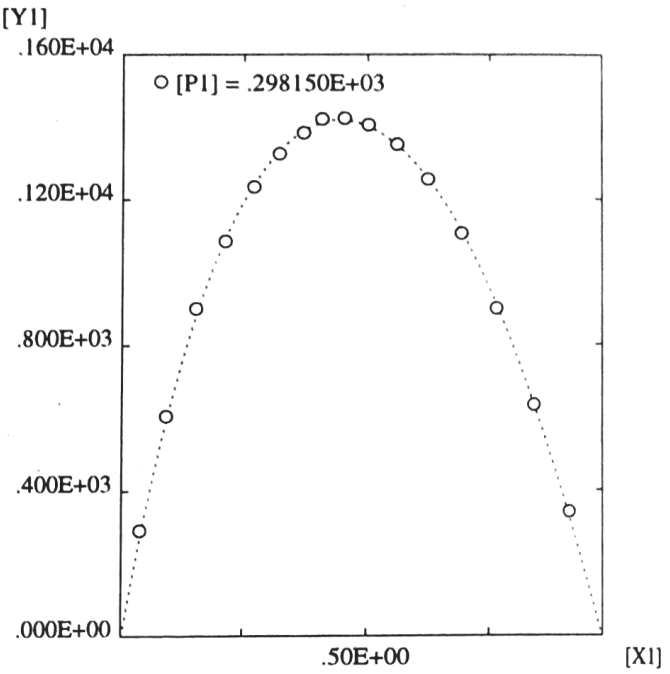
.846400E+00	.634200E+03
.924800E+00	.341400E+03



PLAJ0970.010

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_6H_{12} , Cyclohexane**
2. $C_6H_{12}Br_2$, 1,6-Dibromohexane

[P1] = .298150E+03

[X1]	[Y1]
.786000E–01	.235700E+03
.156200E+00	.450100E+03
.238000E+00	.655900E+03
.314600E+00	.821100E+03
.384300E+00	.940900E+03
.447500E+00	.101280E+04
.502500E+00	.105930E+04
.515500E+00	.107550E+04
.556400E+00	.108090E+04
.602000E+00	.108460E+04
.649800E+00	.104740E+04
.700600E+00	.992700E+03
.752500E+00	.896500E+03
.806000E+00	.766800E+03
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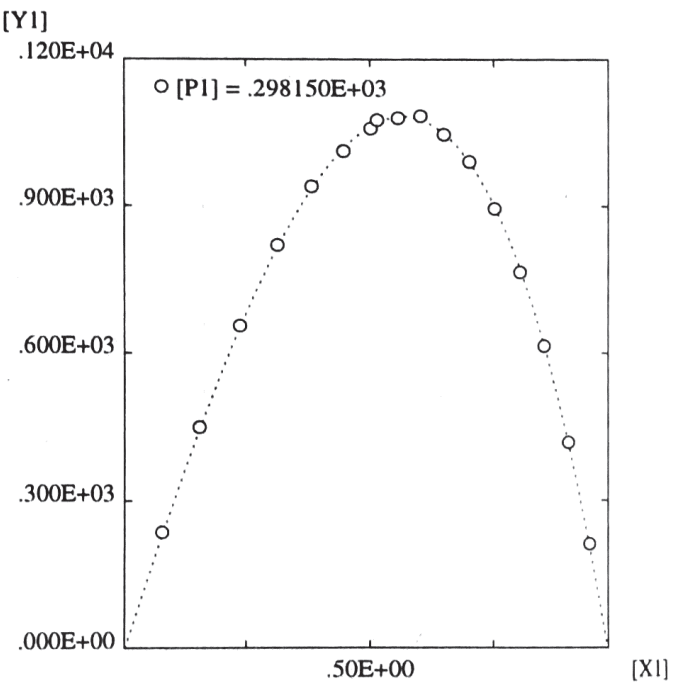
.910400E+00	.418500E+03
.958400E+00	.211500E+03



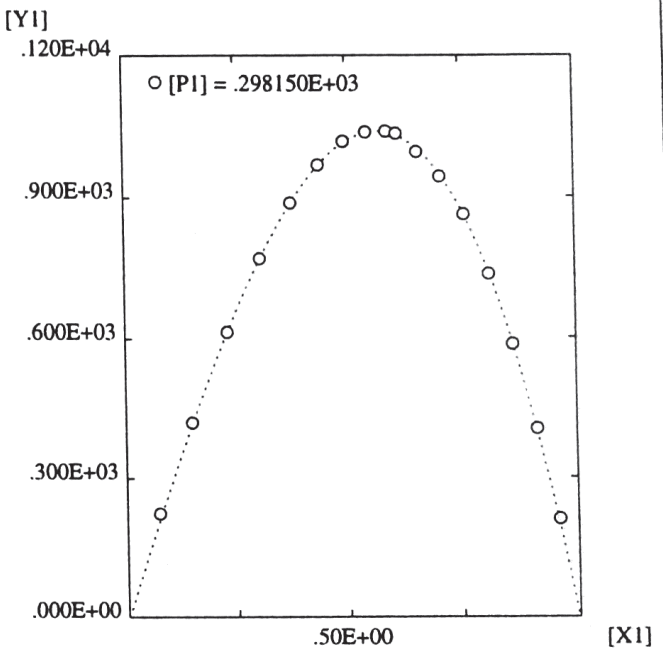
PLAJ0970.005

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_6H_{12} , Cyclohexane**
2. $C_6H_{12}Cl_2$, 1,6-Dichlorohexane

[P1] = .298150E+03

[X1]	[Y1]
.738000E-01	.224400E+03
.151400E+00	.420100E+03
.232800E+00	.614900E+03
.307000E+00	.770600E+03
.377300E+00	.888500E+03
.439800E+00	.970400E+03
.496600E+00	.101990E+04
.546000E+00	.103900E+04
.590700E+00	.104070E+04
.612700E+00	.103530E+04
.659100E+00	.997300E+03
.709300E+00	.943900E+03
.759800E+00	.863400E+03
.814000E+00	.735200E+03
.864000E+00	.586600E+03
.914100E+00	.405000E+03
.959500E+00	.210000E+03



PLAJ0970.014

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_6H_{12} , Cyclohexane**
2. $C_6H_{12}I_2$, 1,6-Diiodohexane

[P1] = .298150E+03

[X1]	[Y1]
.862000E-01	.334700E+03
.167000E+00	.579300E+03
.255600E+00	.824600E+03
.334700E+00	.100900E+04
.408000E+00	.113730E+04
.471700E+00	.121540E+04
.529800E+00	.125740E+04
.550400E+00	.125550E+04
.590300E+00	.124470E+04
.634000E+00	.121500E+04
.678500E+00	.116360E+04
.725900E+00	.108640E+04
.775100E+00	.980200E+03
.825100E+00	.840700E+03
.872400E+00	.676100E+03
.920600E+00	.460600E+03
.961900E+00	.240300E+03