ORTJ0963

ELDATA: Int. Electron. J. Phys.-Chem. Data **1996**, *2*, 121-130

Excess enthalpies of 12 binary liquid mixtures of .alpha.,.omega.-dibromoalkanes (C2, C4, C6) + benzene, toluene, ethylbenzene, or butylbenzene at 298.15 K

Ortega, J.; Placido, J.

Laboratorio de Termodinamica y Fisicoquimica, Escuela Superior de Ingenieros Industriales, Universidad de Las Palmas de Gran Canaria, 35071 – Las Palmas de Gran Canaria, Canary Islands, Spain

(Received in final form February 3, 1997)

Enthalpy-of-mixing H^E measurements are reported at 298.15 K for 12 binary liquid mixtures containing 1,2-dibromoethane, 1,4-dibromobutane, or 1,6-dibromohexane + benzene, + toluene, + ethylbenzene, or + butylbenzene at 298.15 K over the entire range of composition. The H^E curves represented as a function of the mole fraction of dibromoalkane are asymmetrical and may be positive, or negative, or S-shaped. The H^E values are always smaller at low concentrations of the dibromoalkane. They change in the same regular manner with the molecular structure of the components as found previously in the case of α,ω-dichloroalkanes. They decrease from benzene to toluene and then increase with the number of C-atoms of the n-alkylbenzene. For a given n-alkylbenzene, H^E decreases with the number of C-atoms of the dibromoalkane. H^E is the result of an exothermic contribution, due to dipole-induced dipole (n-π) interactions between the polar Br-groups and the π-electrons of the aromatic hydrocarbon, and an endothermic contribution mainly due to dipole-dipole interactions between the polar Br-groups. The more negative H^E with toluene, compared to benzene, is due to the inductive effect of the methyl group in toluene. The endothermic contribution decreases with the number of C-atoms in the dibromoalkane, but increases with the number of C-atoms in the n-alkylbenzene. For a given n-alkylbenzene, the equimolar H^E of an α,ω-dibromoalkane is larger than the equimolar H^E of the α,ω-dichloroalkanes with the same number of C-atoms.

---

1. INTRODUCTION

In continuation of our systematic experimental study on the excess molar enthalpies, H^E, of α,ω-dichloroalkane + aromatic hydrocarbon (benzene, toluene, ethylbenzene, or butylbenzene) mixtures [ORTJ0962], we have determined H^E for 12 systems containing an α,ω-dibromoalkane (1,2-dibromoethane, 1,4-dibromobutane, or 1,6-dibromohexane) + the same aromatic hydrocarbons at 298.15 K. Several H^E data have been published in the literature for 1,2-dibromoethane + benzene, at temperatures from 288.15 to 318.15 K [BAUE1150; BLAS0930; MAHB0760; PERP0830; SPAD0890; SPAD0900], and for 1,2-dibromoethane + toluene, at temperatures from 288.15 to 308.15 K [BAUE1150; SPAD0890; SPAD0900]. We found a single source of data for the series of benzene + α,ω-dibromoalkanes $C_nH_{2n}Br_2$ (n = 1 through 6, and 8) [BLAS0930].

1-Bromoalkane + benzene mixtures have been carefully examined in terms of the DISQUAC group-contribution model [GARN0891]. The study of α,ω-dibromoalkane + n-alkane mixtures [ARTM0914] revealed the occurrence of the Br-Br 'proximity effect' in α,ω-dibromoalkanes and we expect to observe the same effect in α,ω-dibromoalkane + aromatic hydrocarbon mixtures. The H^E database on α,ω-dibromoalkane + n-alkane mixtures has been recently completed [ORTJ0932]. These measurements, along with the data of the present investigation and with literature data on vapor-liquid equilibria, will be used to test the applicability of DISQUAC and other group-contribution models to mixtures of α,ω-dibromoalkanes (and other α,ω-dihaloalkanes) with aromatic hydrocarbons.

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. The temperature T (ITS-90) was maintained constant at (298.15 ± 0.02) K. The microcalorimeter was calibrated electrically after each measurement (see [ORTJ0881]). 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

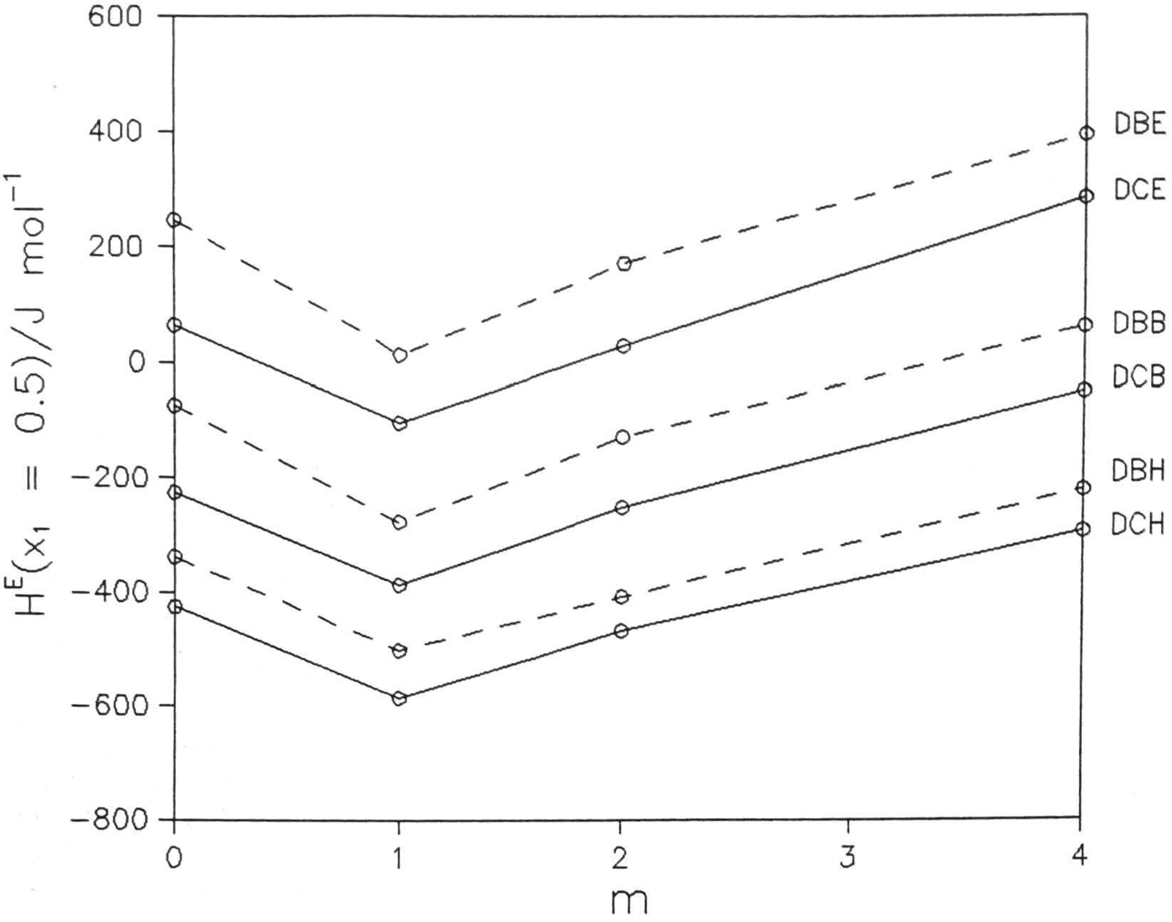


Figure 1. Equimolar excess enthalpies at 298.15 K of 1,2-dibromoethane (DBE), 1,4-dibromobutane (DBB), 1,6-dibromohexane (DBH) (this work) or 1,2-dichloroethane (DCE), 1,4-dichlorobutane (DCB), 1,6-dichlorohexane (DCH) [ORTJ0962] + n-alkylbenzenes: benzene (m = 0), toluene (m = 1), ethylbenzene (m = 2), or butylbenzene (m = 4)

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]).

$C_4H_8Br_2$, 1,4-Dibromobutane. 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) = 1.5167 (1.5169 [TRC00640]); ρ(298.15 K)/kg m^{-3} = 1819.90 (1818.7 [TRC00640]).

C_6H_6, Benzene. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99.8 %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.4980 (1.49792 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 873.51 (873.60 [RIDJ0860]).

$C_6H_{12}Br_2$, 1,6-Dibromohexane. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 97 %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.5054; ρ(298.15 K)/kg m^{-3} = 1602.49.

C_7H_8, Toluene. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99.8 %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.4940 (1.49413 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 862.15 (862.19 [RIDJ0860]).

C_8H_{10}, Ethylbenzene. Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99.8 %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. n(D,298.15 K) = 1.4928 (1.49320 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 862.60 (862.53 [RIDJ0860]).

$C_{10}H_{14}$, Butylbenzene. 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) = 1.4875 (1.48742 [RIDJ0860]); ρ(298.15 K)/kg m^{-3} = 856.17 (856.07 [RIDJ0860]).

3. RESULTS

The direct experimental H^E values are tabulated and graphed in the Appendix and saved on disk as Standard ELDATA Files **`ORTJ0963.001`** through **`ORTJ0963.012`**.

The data were fitted to Eq. (1):

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

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

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

where N is the number of experimental values, are less than 8 J mol^{-1}.

4. DISCUSSION AND CONCLUSIONS

The H^E values at 298.15 K reported in the literature for 1,2-dibromoethane + benzene are in good agreement with our measurements. In the case of 1,2-dibromoethane + toluene the agreement with [BAUE1150] and [SPAD0890] is poor (a difference of ca. 70 J mol^{-1} at equimolar composition and 298.15 K). The largest difference, 240 J mol^{-1} at equimolar composition and 298.15 K, was found in the case of 1,6-dibromohexane + benzene [BLAS0930].

Our H^E results change in the same regular manner with the molecular structure of the components as found previously in the case of α,ω-dichloroalkanes. When represented as a function of the mole fraction of the dibromoalkane, the H^E curves are asymmetrical and may be positive, or negative, or S-shaped. The H^E values are always smaller at low concentrations of the dibromoalkane. They decrease from benzene to toluene and then increase with the number of C-atoms of the n-alkylbenzene. For a given n-alkylbenzene, H^E decreases with the number of C-atoms of the dibromoalkane (Figure 1).

H^E is the result of an exothermic contribution, due to dipole-induced dipole (n-π) interactions between the polar Br-groups and the π-electrons of the aromatic hydrocarbon, and an endothermic contribution mainly due to dipole-dipole interactions between the polar Br-groups. The more negative H^E with toluene, compared to benzene, is due to the inductive effect of the methyl group in toluene. The endothermic contribution decreases with the number of C-atoms in the dibromoalkane, but increases with the number of C-atoms in the n-alkylbenzene.

The H^E values of α,ω-dibromoalkane + n-alkylbenzene mixtures are larger than the H^E values of α,ω-dichloroalkane + n-alkylbenzene mixtures [ORTJ0962] (Figure 1).

REFERENCES

[ARTM0914] – Artal, M.; Munoz Embid, J.; Otin, S.; Velasco, I.; Kehiaian, H. V. Excess enthalpies of binary mixtures containing .alpha.,.omega.-dibromoalkanes. Measurement and analysis in terms of group contributions (DISQUAC). *Fluid Phase Equilib.* **1991,** *70,* 267-274.

[BAUE1150] – Baud, E. Analyse thermique des melanges binaires. *Bull. Soc. Chim. Fr.* **1915,** *17,* 329-345.

[BLAS0930] – Blanco, S.; Artal, M.; Fernandez, J.; Munoz Embid, J.; Otin, S. Excess enthalpies of dibromoalkane + benzene binary mixtures at 298.15 K. *J. Chem. Eng. Data* **1993,** *38,* 587-588.

[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.

[GARN0891] – Garcia-Lisbona, N.; Garcia Vicente, I.; Munoz Embid, J.; Velasco, I.; Otin, S.; Kehiaian, H. V. Thermodynamics of mixtures containing bromoalkanes. II. Excess enthalpies of of mixtures of 1-bromoalkane with cyclohexane, with benzene, or with tetrachloromethane. Measurement and analysis in terms of group contributions (DISQUAC). *Fluid Phase Equilib.* **1989,** *45,* 191-203.

[MAHB0760] – Mahl, B. S.; Kooner, Z. S.; Khurma, J. R. Thermodynamics of binary mixtures: excess enthalpies of 1,2-dibromoethane mixtures with benzene, cyclohexane, carbon tetrachloride and dioxane at 25.deg.C. *Thermochim. Acta* **1976,**, 256-259.

[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.

[ORTJ0881] – Ortega, J.; Matos, J. S.; Paz Andrade, M. I.; Fernandez, J.; Pias, L. Analysis of excess enthalpies of ester + 1-bromoalkanes with two group contribution models: primary parameters. *Fluid Phase Equilib.* **1988,** *43,* 295-316.

[ORTJ0932] – Ortega, J.; Placido, J. Excess enthalpies of some .alfa.,.omega.-dibromoalkane (C2-C6) + normal alkane (C5-C7) mixtures. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1993,** *21,* 48-84.

[ORTJ0962] – Ortega, J.; Placido, J. Excess enthalpies of 12 binary liquid mixtures of .alpha.,.omega.-dichloroalkanes (C2, C4, C6) + aromatic hydrocarbons (benzene, toluene, ethylbenzene, or butylbenzene) at 298.15 K. *ELDATA Int. Electron. J. Phys.-Chem. Data* **1996,** *2,* 111-120.

[PERP0830] – Perez, P.; Florian, A.; Lazaro, A.; Gracia, M.; Gutierrez Losa, C.; Valero, J. Conformational equilibrium and its influence on the dielectric and thermodynamic behaviour of cyclohexane or benzene + 1,2-dibromoethane. *Ber. Bunsen-Ges. Phys. Chem.* **1983,** *87,* 5-10.

[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.

[SPAD0890] – Spah, D. C.; Verma, P. K.; Singh, K. C.; Kalra, K. C. Excess volumes of mixing and excess enthalpies of mixing of 1,2-dibromoethane with aromatic hydrocarbons at 298.15 K. *Thermochim. Acta* **1989,** *146,* 187-199.

[SPAD0900] – Spah, D. C.; Singh, K. C.; Kalra, K. C. Thermodynamics of molecular interactions of 1,2-dibromoethane + aromatic hydrocarbon mixtures at 308.15 K. *Indian J. Chem., Sect. A.* **1990,** *29,* 546-551.

[TRC00640] – TRC. *TRC Thermodynamic Tables - Non-Hydrocarbons.* Thermodynamics Research Center, Texas A&M University System, College Station, TX, USA (loose-leaf data sheets extant) **1964,** a-7580.

Ortega, Juan* [ORTJ0]
Placido, Jose [PLAJ0]

*Author to whom correspondence should be addressed:

FAX +34-28-363859

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.001**

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

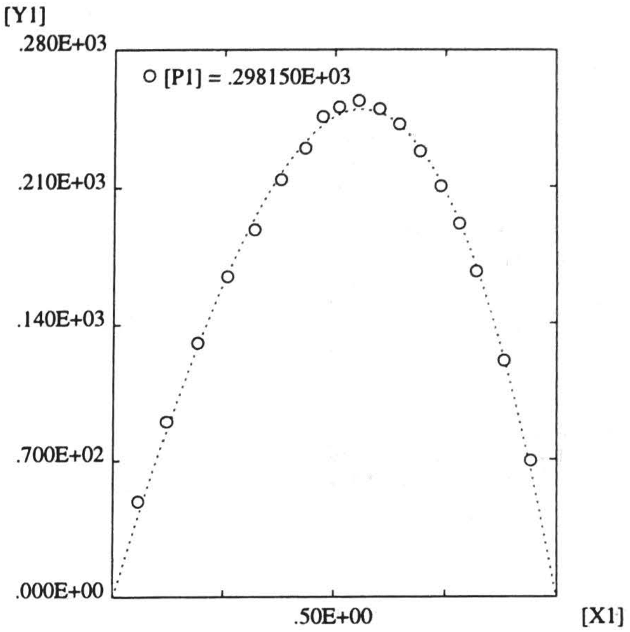
Parameters: [P1] T/K, Temperature

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. $C_2H_4Br_2$, 1,2-Dibromoethane**
2. C_6H_6 , Benzene

[P1] = .298150E+03	
[X1]	[Y1]
.585000E–01	.492000E+02
.123000E+00	.901000E+02
.191100E+00	.130800E+03
.258100E+00	.164800E+03
.320300E+00	.188600E+03
.379200E+00	.214200E+03
.433900E+00	.230000E+03
.473300E+00	.245900E+03
.510800E+00	.250800E+03
.553800E+00	.253800E+03
.601500E+00	.249900E+03
.646100E+00	.242200E+03
.692700E+00	.228500E+03
.740300E+00	.210400E+03
.781600E+00	.191300E+03
.819600E+00	.166800E+03
.881300E+00	.121000E+03
.943700E+00	.693000E+02



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.002**

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

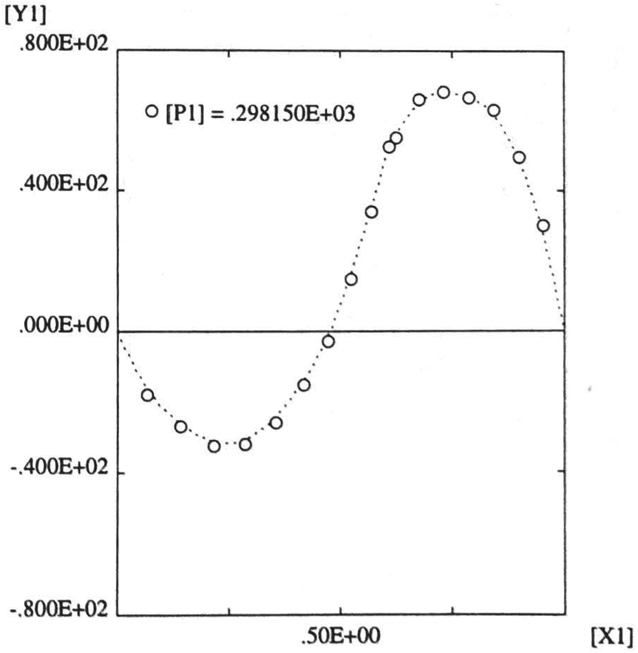
Parameters: [P1] T/K, Temperature

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. $C_2H_4Br_2$, 1,2-Dibromoethane**
2. C_7H_8 , Toluene

[P1] = .298150E+03	
[X1]	[Y1]
.686000E–01	–.178000E+02
.142100E+00	–.267000E+02
.215900E+00	–.322000E+02
.286800E+00	–.320000E+02
.355000E+00	–.258000E+02
.417300E+00	–.152000E+02
.473400E+00	–.270000E+01
.523500E+00	.148000E+02
.568800E+00	.340000E+02
.609800E+00	.527000E+02
.626500E+00	.552000E+02
.677500E+00	.662000E+02
.731800E+00	.683000E+02
.788600E+00	.667000E+02
.845100E+00	.631000E+02
.901300E+00	.497000E+02
.954200E+00	.300000E+02



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.003**

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

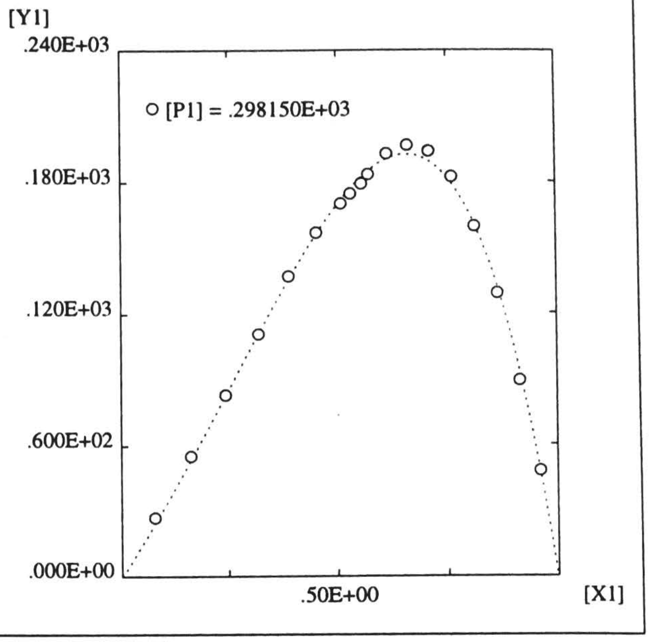
Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] 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_8H_{10} , Ethylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.793000E–01	.272000E+02
.163100E+00	.552000E+02
.245300E+00	.832000E+02
.320900E+00	.110900E+03
.390500E+00	.137200E+03
.453300E+00	.157000E+03
.510600E+00	.170300E+03
.531900E+00	.174700E+03
.556800E+00	.179100E+03
.572400E+00	.183400E+03
.615200E+00	.192600E+03
.661600E+00	.196600E+03
.710300E+00	.193900E+03
.761600E+00	.182100E+03
.813900E+00	.159900E+03
.864600E+00	.129100E+03
.914100E+00	.893000E+02
.959600E+00	.481000E+02



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.004**

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

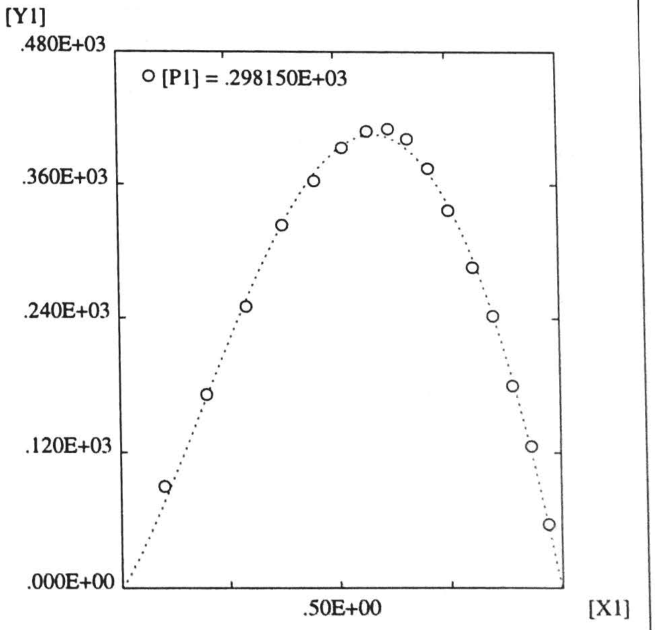
Parameters: [P1] T/K, Temperature

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. $C_2H_4Br_2$, 1,2-Dibromoethane**
2. $C_{10}H_{14}$, Butylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.100200E+00	.902000E+02
.200800E+00	.172100E+03
.295100E+00	.250300E+03
.378500E+00	.323900E+03
.454000E+00	.363800E+03
.517900E+00	.394000E+03
.574200E+00	.408600E+03
.622800E+00	.410600E+03
.664700E+00	.401800E+03
.710800E+00	.375100E+03
.754200E+00	.337700E+03
.807000E+00	.286800E+03
.851100E+00	.242900E+03
.893400E+00	.180000E+03
.933500E+00	.126400E+03
.970400E+00	.568000E+02

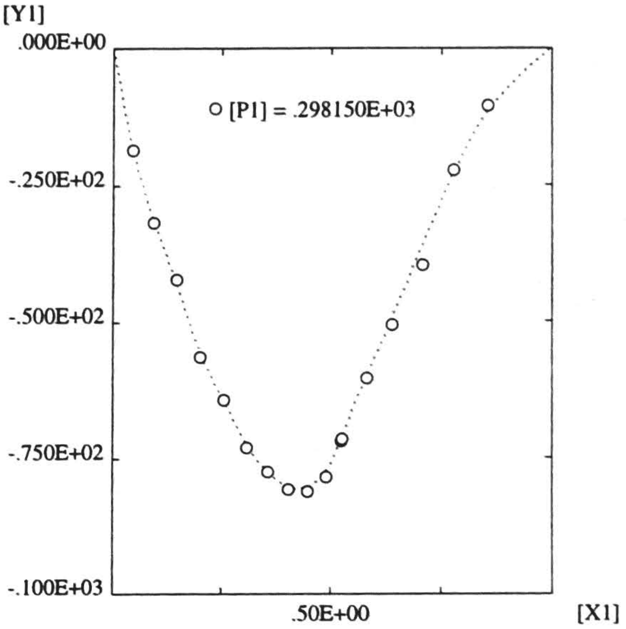


ORTJ0963.005

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. $C_4H_8Br_2$, 1,4-Dibromobutane**
2. C_6H_6 , Benzene

[P1] = .298150E+03			
[X1]	[Y1]		
.459000E–01	–.184000E+02		
.951000E–01	–.317000E+02		
.148000E+00	–.422000E+02		
.201700E+00	–.563000E+02		
.257200E+00	–.642000E+02		
.309500E+00	–.730000E+02		
.358900E+00	–.774000E+02		
.405400E+00	–.807000E+02		
.449400E+00	–.811000E+02		
.490700E+00	–.785000E+02		
.525200E+00	–.718000E+02		
.528100E+00	–.715000E+02		
.583500E+00	–.603000E+02		
.639700E+00	–.506000E+02		
.708400E+00	–.397000E+02		
.778700E+00	–.222000E+02		
.855900E+00	–.105000E+02		

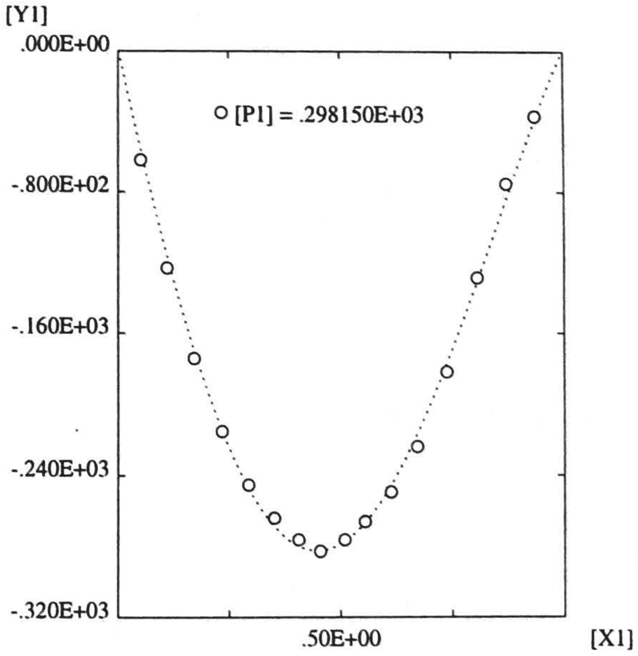


ORTJ0963.006

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. $C_4H_8Br_2$, 1,4-Dibromobutane**
2. C_7H_8 , Toluene

[P1] = .298150E+03			
[X1]	[Y1]		
.516000E–01	–.619000E+02		
.111300E+00	–.122900E+03		
.172600E+00	–.174100E+03		
.234700E+00	–.214800E+03		
.295300E+00	–.244800E+03		
.352500E+00	–.263800E+03		
.406600E+00	–.276200E+03		
.456200E+00	–.282700E+03		
.510600E+00	–.276300E+03		
.556000E+00	–.265900E+03		
.612800E+00	–.248800E+03		
.672700E+00	–.223400E+03		
.737800E+00	–.181300E+03		
.806600E+00	–.128200E+03		
.873000E+00	–.749000E+02		
.936900E+00	–.364000E+02		



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.007**

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

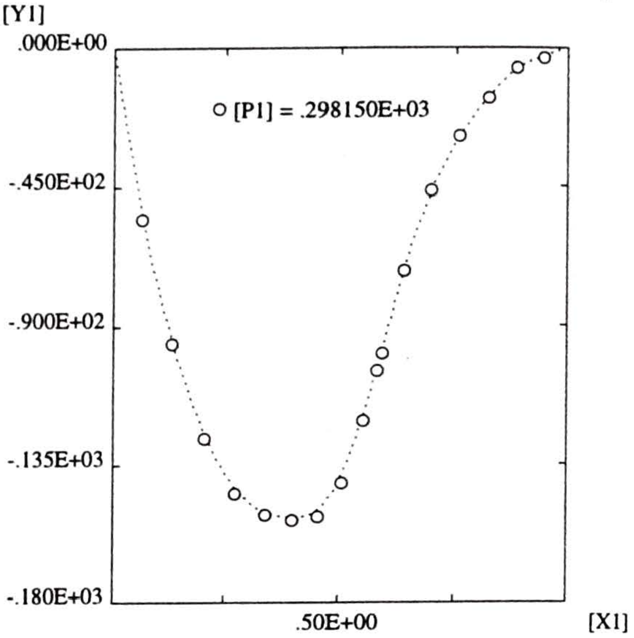
Parameters: [P1] T/K, Temperature

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. $C_4H_8Br_2$, 1,4-Dibromobutane**
2. C_8H_{10} , Ethylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.645000E–01	–.553000E+02
.134000E+00	–.956000E+02
.206600E+00	–.126300E+03
.276500E+00	–.144400E+03
.342500E+00	–.151300E+03
.402400E+00	–.153100E+03
.458500E+00	–.151900E+03
.508800E+00	–.141000E+03
.553700E+00	–.120700E+03
.584300E+00	–.104600E+03
.593900E+00	–.990000E+02
.639100E+00	–.721000E+02
.697200E+00	–.463000E+02
.759300E+00	–.287000E+02
.822600E+00	–.162000E+02
.885600E+00	–.630000E+01
.946700E+00	–.320000E+01



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.008**

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

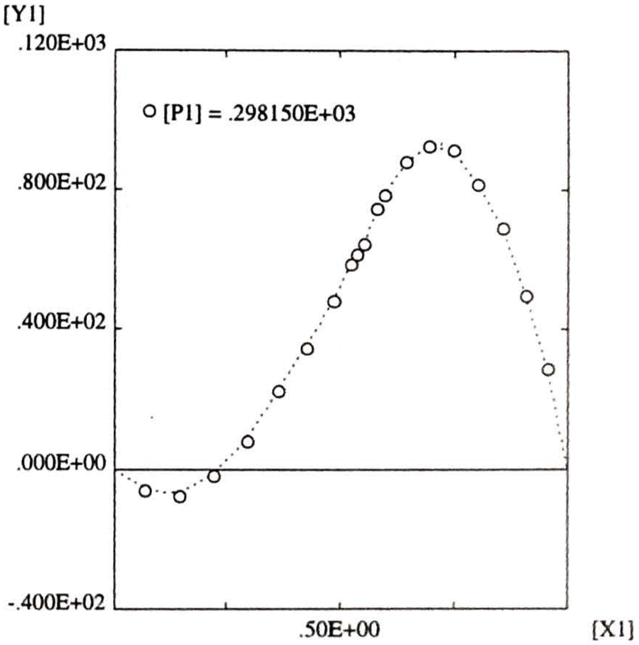
Parameters: [P1] T/K, Temperature

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. $C_{10}H_{14}$, Butylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.697000E–01	–.590000E+01
.147100E+00	–.750000E+01
.224200E+00	–.160000E+01
.299400E+00	.820000E+01
.367700E+00	.222000E+02
.430300E+00	.346000E+02
.487600E+00	.481000E+02
.525800E+00	.587000E+02
.537800E+00	.616000E+02
.553800E+00	.646000E+02
.582800E+00	.747000E+02
.598600E+00	.786000E+02
.646600E+00	.881000E+02
.696600E+00	.927000E+02
.748600E+00	.915000E+02
.802600E+00	.817000E+02
.856400E+00	.691000E+02
.909300E+00	.498000E+02
.957800E+00	.285000E+02



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.009**

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

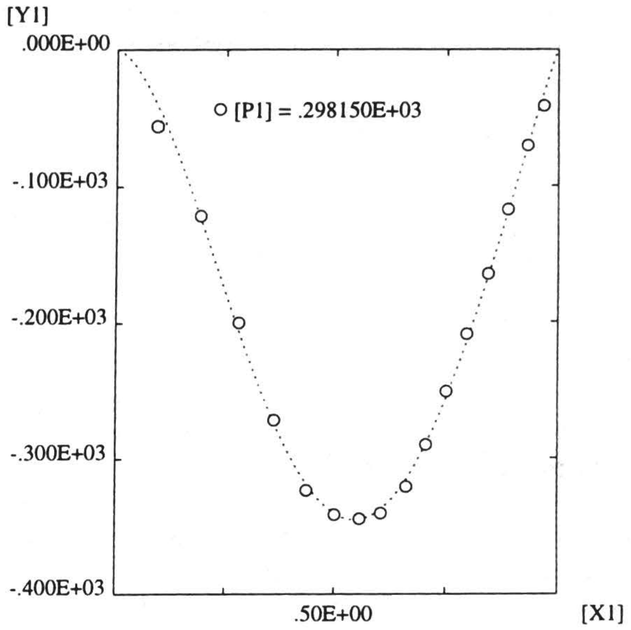
Parameters: [P1] T/K, Temperature

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_6H_6 , Benzene**
2. $C_6H_{12}Br_2$, 1,6-Dibromohexane

[P1] = .298150E+03			
[X1]	[Y1]		
.930000E–01	–.559000E+02		
.192900E+00	–.121500E+03		
.282800E+00	–.199600E+03		
.363300E+00	–.271100E+03		
.438000E+00	–.323200E+03		
.502200E+00	–.341200E+03		
.559300E+00	–.344300E+03		
.607700E+00	–.340300E+03		
.663900E+00	–.320700E+03		
.707400E+00	–.289900E+03		
.752700E+00	–.250700E+03		
.798300E+00	–.209000E+03		
.844400E+00	–.164600E+03		
.889000E+00	–.117200E+03		
.931500E+00	–.704000E+02		
.968000E+00	–.413000E+02		



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION **ORTJ0963.010**

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

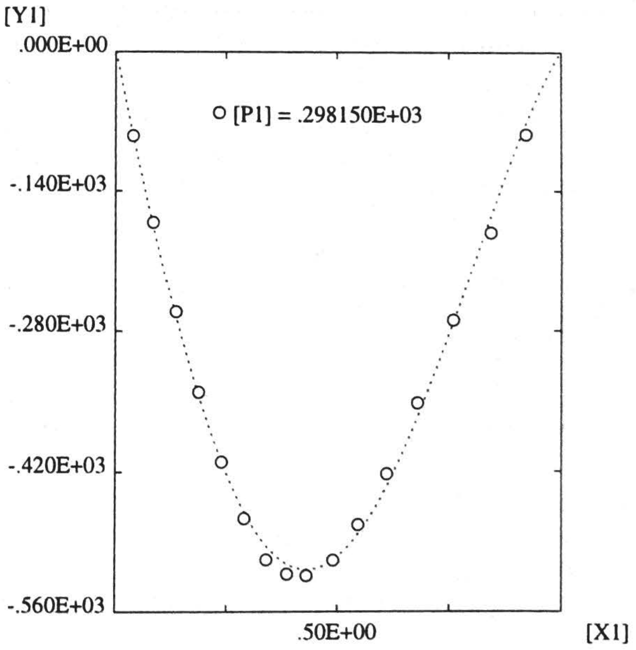
Parameters: [P1] T/K, Temperature

Variables: [X1] x_1/-, Mole fraction of component 1
[Y1] 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. $C_6H_{12}Br_2$, 1,6-Dibromohexane**
2. C_7H_8 , Toluene

[P1] = .298150E+03			
[X1]	[Y1]		
.415000E–01	–.847000E+02		
.863000E–01	–.170900E+03		
.136500E+00	–.259800E+03		
.188100E+00	–.340400E+03		
.240300E+00	–.410000E+03		
.291300E+00	–.465600E+03		
.341200E+00	–.507500E+03		
.387600E+00	–.521900E+03		
.431800E+00	–.522900E+03		
.490700E+00	–.508100E+03		
.548300E+00	–.472200E+03		
.611600E+00	–.422000E+03		
.680400E+00	–.351900E+03		
.760400E+00	–.268200E+03		
.843000E+00	–.181100E+03		
.922700E+00	–.826000E+02		

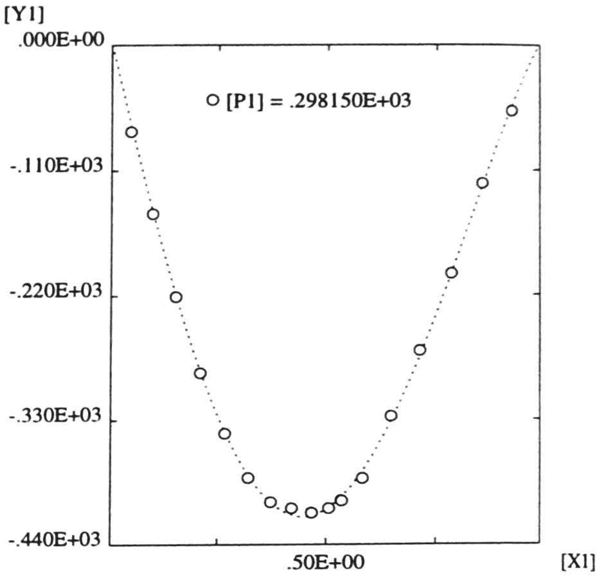


ORTJ0963.011

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. $C_6H_{12}Br_2$, 1,6-Dibromohexane**
2. C_8H_{10} , Ethylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.458000E–01	–.758000E+02
.978000E–01	–.147500E+03
.152900E+00	–.221000E+03
.210200E+00	–.288000E+03
.267300E+00	–.341900E+03
.323200E+00	–.380900E+03
.374800E+00	–.402100E+03
.422200E+00	–.407900E+03
.467200E+00	–.411700E+03
.507700E+00	–.407800E+03
.535200E+00	–.400800E+03
.536200E+00	–.401500E+03
.582900E+00	–.381200E+03
.647500E+00	–.327000E+03
.713700E+00	–.269500E+03
.785600E+00	–.201400E+03
.859200E+00	–.121900E+03
.931100E+00	–.581000E+02



ORTJ0963.012

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. $C_6H_{12}Br_2$, 1,6-Dibromohexane**
2. $C_{10}H_{14}$, Butylbenzene

[P1] = .298150E+03	
[X1]	[Y1]
.594000E–01	–.517000E+02
.126700E+00	–.997000E+02
.193100E+00	–.143600E+03
.259700E+00	–.178800E+03
.322300E+00	–.205300E+03
.380200E+00	–.225400E+03
.457900E+00	–.231200E+03
.499300E+00	–.233500E+03
.544000E+00	–.225300E+03
.593200E+00	–.207700E+03
.647200E+00	–.179800E+03
.704200E+00	–.145300E+03
.764800E+00	–.114500E+03
.825500E+00	–.878000E+02
.889700E+00	–.525000E+02
.946900E+00	–.269000E+02