

Excess enthalpies of 12 binary liquid mixtures of trichloromethane or 1,1,2,2-tetrachloroethane + 1-chloroalkanes (C4 - C9) at 298.15 K

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Enthalpy-of-mixing, H^E , measurements are reported at 298.15 K for 1-chloroalkanes (1-chlorobutane through 1-chlorononane) + trichloromethane or + 1,1,2,2-tetrachloroethane. The mixtures containing 1-chlorobutane are exothermic. H^E increases with the chain length of the 1-chloroalkane becoming negative/positive or positive for 1,1,2,2-tetrachloroethane + 1-chlorooctane or + 1-chlorononane. The experimental H^E data are not reproduced by the Modified UNIFAC group contribution method (Dortmund version), using the parameters published in 1993, mainly because of having neglected the group proximity effect. The DISQUAC model, with dispersive parameters changing regularly with the structure of the molecules, describes fairly well both the magnitude and the shape of the experimental H^E curves.

1. INTRODUCTION

In continuation of our systematic experimental studies on the excess molar enthalpies H^E of trichloromethane or 1,1,2,2-tetrachloroethane + n-alkanes [ORTJ0952; ORTJ0953], we have determined H^E of the same two solvents + 1-chloroalkanes (1-chlorobutane through 1-chlorononane). No H^E data are available in the literature on these classes of mixtures, except for 1-chlorobutane [MUNJ0901]. These data have been compared with the predictions of the Modified UNIFAC Model [WEIU0871; GMEJ0930] and have been used to estimate new interchange parameters for the DISQUAC group-contribution model [KEHH0830].

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 cm³) and with negligible vapor phase [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 [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 $\sigma(H^E) = 0.5 \text{ J mol}^{-1} + 0.02 |H^E|$.

2.2. Materials

CHCl₃, Trichloromethane (Chloroform). Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4429$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 1480.03$.

C₂H₂Cl₄, 1,1,2,2-Tetrachloroethane Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4918$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 1588.37$.

C₄H₉Cl, 1-Chlorobutane (Butyl chloride). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated GLC purity > 99.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.3997$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 880.29$.

C₅H₁₁Cl, 1-Chloropentane (Amyl chloride). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated GLC purity > 99.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4099$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 876.92$.

C₆H₁₃Cl, 1-Chlorohexane (Hexyl chloride). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated GLC purity > 99.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4174$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 873.33$.

C₇H₁₅Cl, 1-Chloroheptane (Heptyl chloride). ALFA Products (Danvers, MA, USA) material of stated purity

> 99.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4232$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 870.56$.

C₈H₁₇Cl, 1-Chlorooctane (Octyl chloride). Fluka AG (Buchs, Switzerland) "puriss" grade material of stated GLC purity > 98.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4280$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 868.65$.

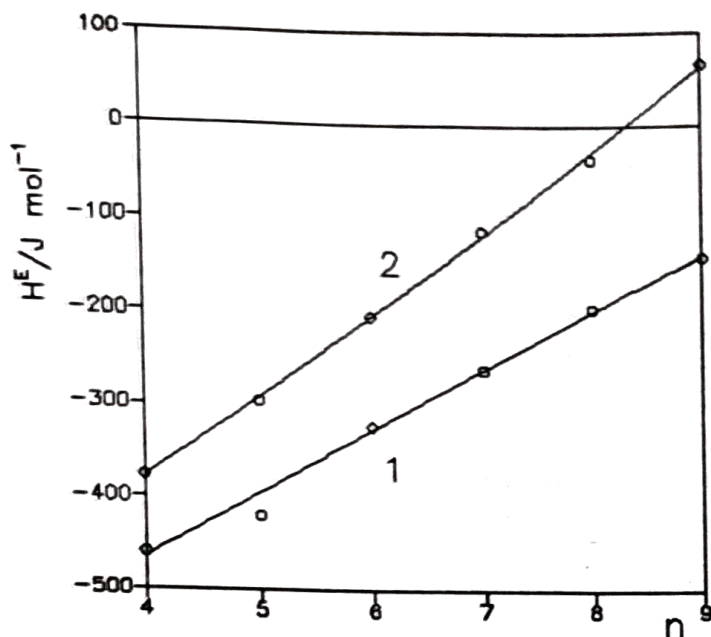


Figure 1. Change of the equimolar excess enthalpy H^E at 298.15 K of trichloromethane or 1,1,2,2-tetrachloroethane + 1-chloroalkanes, $C_nH_{2n+1}Cl$, with the number n of C atoms in the 1-chloroalkanes: 1 – trichloromethane; 2 – 1,1,2,2-tetrachloroethane. Points, experimental data (this work); curves, DISQUAC calculation

C₉H₁₉Cl, 1-Chlorononane (Nonyl chloride). Aldrich Chem. Co., Inc. (Milwaukee, WI, USA) material of stated purity > 99.0 mole %, was degassed ultrasonically, dried over molecular sieves Type 3A (reference 69828, from Fluka), and used without further purification. $n(D, 298.15 \text{ K}) = 1.4324$; $\rho_i(298.15 \text{ K})/\text{kg m}^{-3} = 867.74$.

3. RESULTS

The direct experimental H^E values are tabulated and graphed in the Appendix and saved on disk as Standard ELDATA Files **PLAJ0950.001** through **PLAJ0950.012**.

The data were fitted to Eq. (1):

$$H^E_{\text{calc}}/\text{J mol}^{-1} = x_1 x_2 \sum A_i [x_1/(x_1 + kx_2)]^{i-1} \quad (1)$$

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):

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

where N is the number of experimental values, are less than 7.5 J mol^{-1} .

At equimolar composition, our H^E values for 1-chlorobutane + trichloromethane or + 1,1,2,2-tetrachloroethane differ by as much as ca. 100 J mol^{-1} from the values reported by [MUNJ0950].

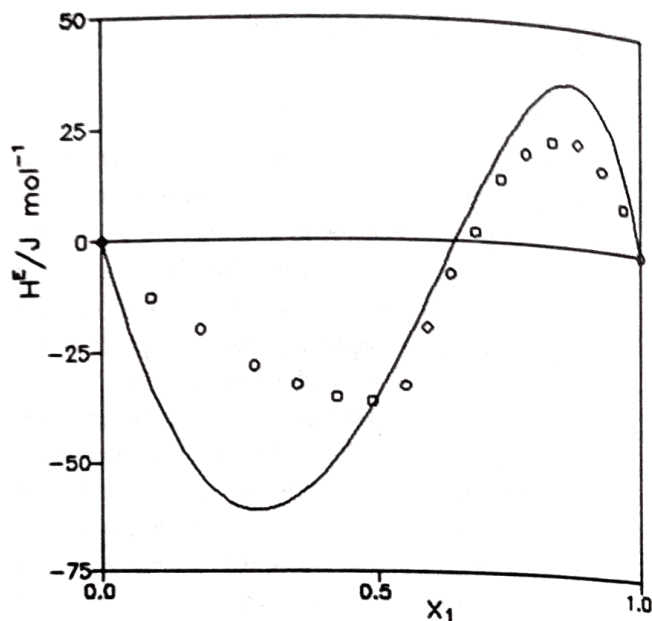


Figure 2. Excess molar enthalpy H^E of 1,1,2,2-tetrachloroethane + 1-chlorooctane at 298.15 K as a function of the mole fraction x_1 of 1,1,2,2-tetrachloroethane. Points, experimental data (this work); curve, DISQUAC calculation

4. DISCUSSION AND CONCLUSIONS

The excess enthalpies of 1-chlorobutane + trichloromethane or + 1,1,2,2-tetrachloroethane are negative and increase with the chain length of the 1-chloroalkane (Fig. 1). 1,1,2,2-Tetrachloroethane + 1-chlorooctane has an S-shaped H^E curve (Fig. 2) and for 1,1,2,2-tetrachloroethane + 1-chlorononane H^E is positive.

The Modified UNIFAC model [WEIU0871] provides interaction parameters for all the groups involved in mixtures containing 1-chloroalkanes, trichloromethane, and 1,1,2,2-tetrachloroethane [GMEJ0930]. However, the predicted H^E values differ considerably from the experimental ones. E. g., at 298.15 K, the calculated equimolar H^E values for 1-chlorobutane + trichloromethane or + 1,1,2,2-tetrachloroethane are, respectively, -231 and 173 J mol^{-1} , whereas the

experimental are -460 and -377 J mol⁻¹. Similarly, for 1-chlorooctane + trichloromethane or + 1,1,2,2-tetrachloroethane the calculated equimolar H^E values are, respectively, -73 and 506 J mol⁻¹, whereas the experimental are -195 and -35 J mol⁻¹.

The reason of these discrepancies is, besides the lack of appropriate experimental H^E data, mainly the difficulty to define a unique set of functional groups for halogenated hydrocarbons in the frame of UNIFAC [WUOH0910]. In polychloroalkanes, like in many other polyfunctional molecules, the electrical charge distribution on the Cl atoms depends on the proximity of these atoms on the different molecules [WUOH0910]. Consequently, the interaction parameters, of any group contribution method, change with the structure of the molecules. In order to obtain better fits with the UNIFAC method, it appears to be necessary to define additional subgroups and determine the corresponding parameters using new experimental H^E data.

The DISQUAC model [KEHH0830] has been applied to investigate the proximity effect in several chloroalkane mixtures [KEHH0880; KEHH0881; MUNJ0902; MUNJ0910]. Chloroalkanes are regarded as consisting of two types of groups or contact surfaces s,t: (i) type a – aliphatic (CH₃, CH₂, or CH) and (ii) type d – chlorine (Cl). The aliphatic groups are assumed to exert the same force field with respect to Cl groups independent of the chloroalkane. In the chloroalkanes under investigation, we distinguish three types of Cl atoms: d – in 1-chloroalkanes, d' – in trichloromethane, and d'' – in 1,1,2,2-tetrachloroethane. The geometrical parameters (relative volumes and surfaces and surface fractions) of these groups and molecules, as well as the dispersive and quasichemical coefficients $C_{st,l}^{DIS}$ and $C_{st,l}^{QUAC}$ ($l = 1$, Gibbs energy; $l = 2$, enthalpy) of (ad), (ad'), and (ad'') contacts, have been determined previously [KEHH0881]. The same coefficients have been used now. As in many other cases, we assumed that the quasichemical coefficients of the polar-polar contacts (dd') and (dd'') are equal to zero. We fitted the dispersive enthalpic interchange coefficients, $C_{st,2}^{DIS}$, to the experimental equimolar H^E values. The coefficient of trichloromethane (st = dd') decreases slightly with the number n of C atoms in the 1-chloroalkanes (Figure 3, curve 1) from -0.86 ($n = 4$) to -0.95 ($n = 8$). The decrease is much stronger in the case of 1,1,2,2-tetrachloroethane (st = dd'') (Figure 3, curve 2), from -1.34 ($n = 4$) to -2.10 ($n = 8$). We found previously, for 1-chloroalkanes + tetrachloromethane [KEHH0881], a slight increase of the dispersive enthalpic interchange coefficient. The shapes of the H^E curves as a function of the mole fraction x_1 are fairly well represented over the entire composition range (see, e. g., Figure 2).

Experimental vapor-liquid equilibrium data are needed to estimate the dispersive Gibbs energy interchange coefficients, $C_{st,1}^{DIS}$. Unfortunately, no such data have been reported in the literature for trichloromethane or

1,1,2,2-tetrachloroethane + any 1-chloroalkane [WICI0930; WICI0950].

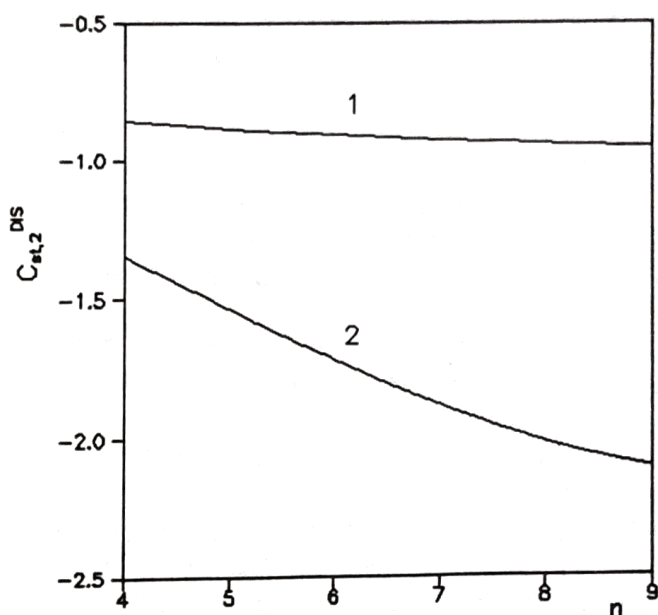


Figure 3. Change of the dispersive enthalpic interchange coefficients, $C_{st,2}^{DIS}$, with the number n of C atoms in the 1-chloroalkane: 1 – trichloromethane (st = dd'); 2 – 1,1,2,2-tetrachloroethane (st = dd'')

Acknowledgements

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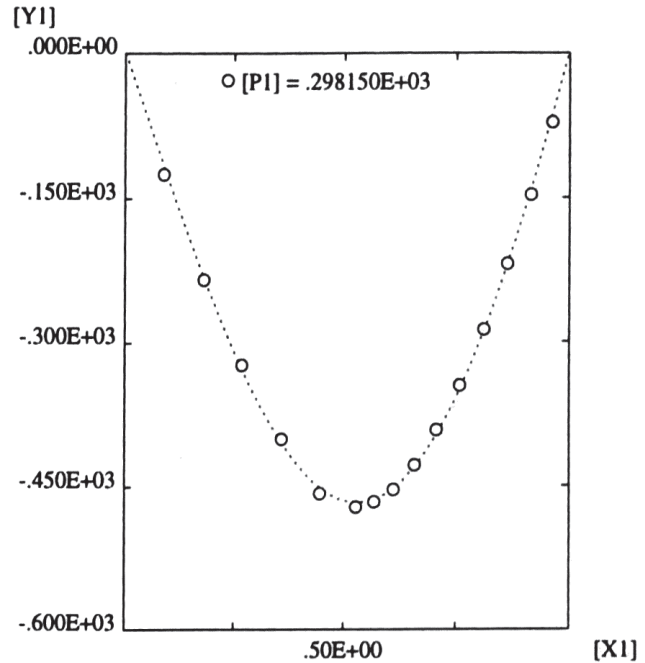
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Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
 State: Two-component system, single-phase liquid or two-phase liquid-liquid (LL)
 Pure component 1, liquid
 Pure component 2, liquid
 Parameters: [P1] T/K, Temperature
 Variables: [X1] x_1 /-, 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

PLAJ0950.001

Components: 1. CHCl₃, Trichloromethane
 2. C₄H₉Cl, 1-Chlorobutane

[P1] = .298150E+03	
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.182800E+00	-.234700E+03
.270100E+00	-.322700E+03
.359600E+00	-.399800E+03
.448300E+00	-.457500E+03
.528700E+00	-.471100E+03
.569900E+00	-.465900E+03
.613900E+00	-.453200E+03
.659400E+00	-.427600E+03
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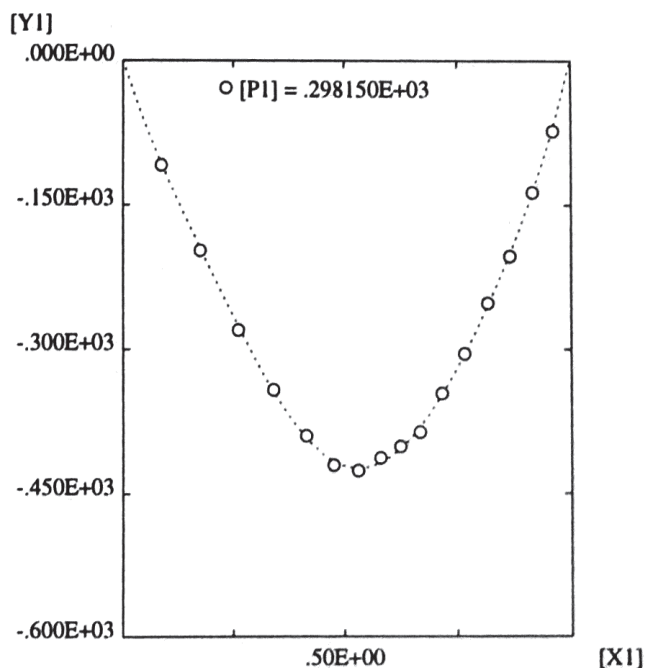


Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION
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 Pure component 1, liquid
 Pure component 2, liquid
 Parameters: [P1] T/K, Temperature
 Variables: [X1] x_1 /-, Mole fraction of component 1
 [Y1] H^E /J mol⁻¹, Molar excess enthalpy
 Method: Direct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

PLAJ0950.002

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 2. C₅H₁₁Cl, 1-Chloropentane

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.341400E+00	-.342000E+03
.414500E+00	-.389000E+03
.475500E+00	-.419400E+03
.531200E+00	-.425900E+03
.580500E+00	-.412300E+03
.623600E+00	-.400100E+03
.667900E+00	-.385400E+03
.716000E+00	-.345200E+03
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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. CHCl₃, Trichloromethane2. C₆H₁₃Cl, 1-Chlorohexane

[P1] = .298150E+03

[X1]

[Y1]

.871000E-01	-.828000E+02
.180100E+00	-.152800E+03
.269700E+00	-.218500E+03
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.547600E+00	-.335100E+03
.596100E+00	-.340500E+03
.638500E+00	-.339800E+03
.675900E+00	-.335100E+03
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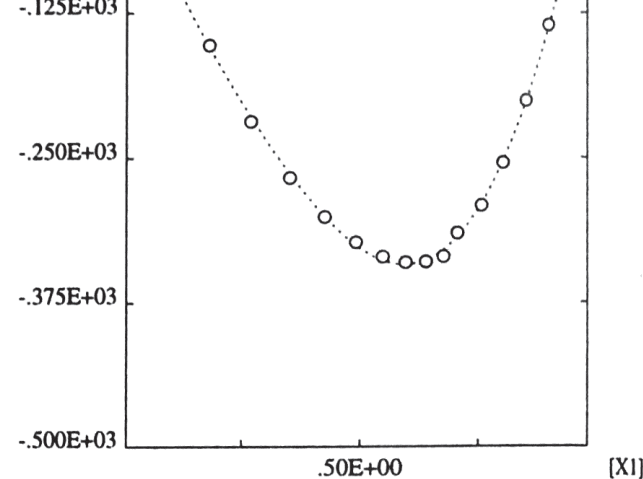
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○ [P1] = .298150E+03

**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. CHCl₃, Trichloromethane2. C₇H₁₅Cl, 1-Chloroheptane

[P1] = .298150E+03

[X1]

[Y1]

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.529900E+00	-.269800E+03
.584300E+00	-.277800E+03
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.741700E+00	-.249000E+03
.782000E+00	-.227800E+03
.822000E+00	-.201800E+03
.862900E+00	-.166200E+03
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[Y1]

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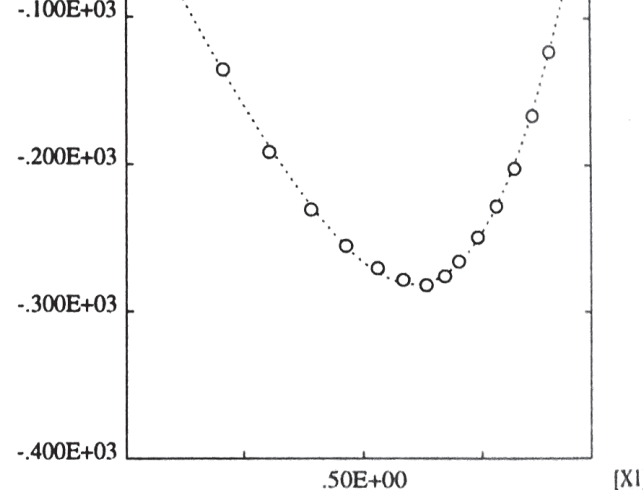
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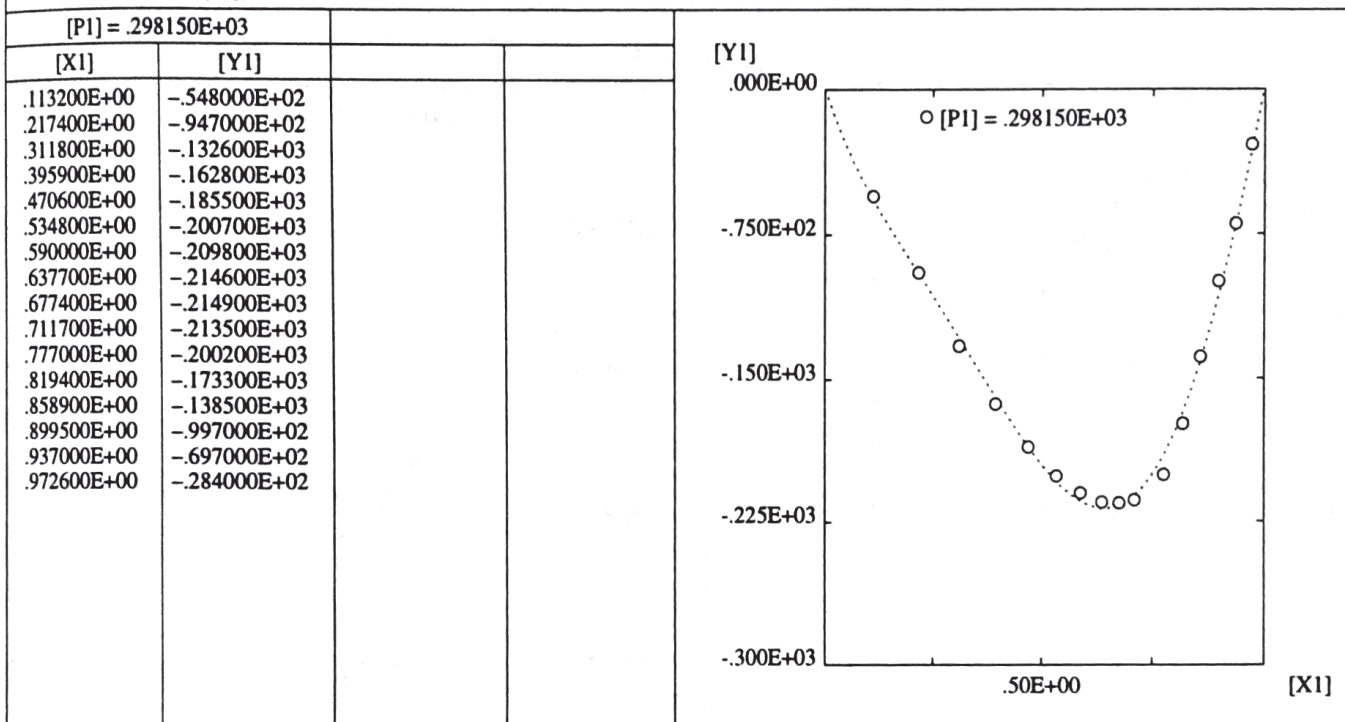
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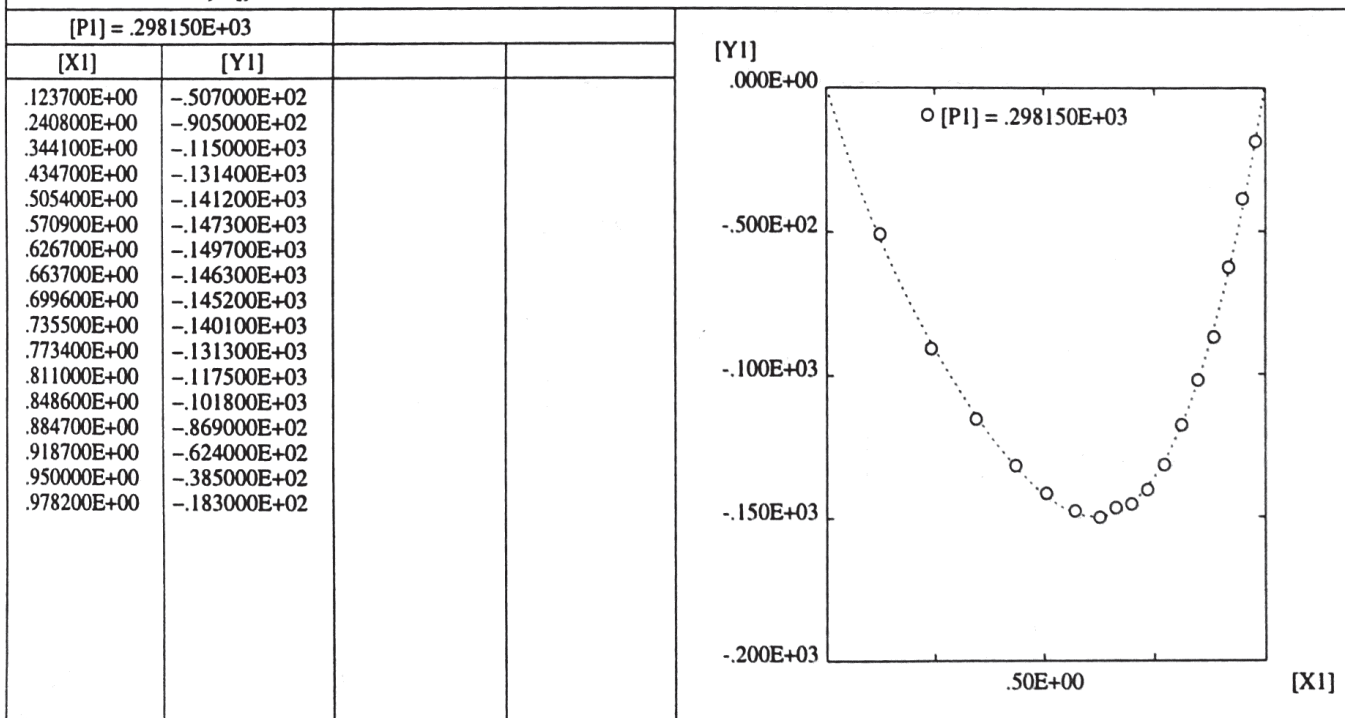
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Method: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T	

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2. C₈H₁₇Cl, 1-Chlorooctane



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION	PLAJ0950.006
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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. CHCl₃, Trichloromethane
2. C₉H₁₉Cl, 1-Chlorononane



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION

PLAJ0950.007

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

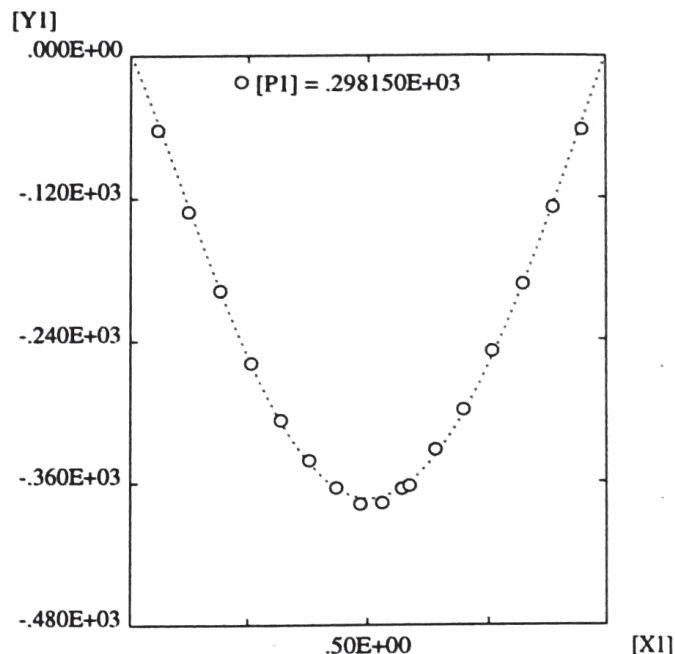
Parameters: [P1] T/K, Temperature

Variables: [X1] x_1 /-, Mole fraction of component 1[Y1] H^E /J mol⁻¹, Molar excess enthalpyMethod: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: 1. C₂H₂Cl₄, 1,1,2,2-Tetrachloroethane
 2. C₄H₉Cl, 1-Chlorobutane

[P1] = .298150E+03

[X1]	[Y1]
.584000E-01	-.624000E+02
.124400E+00	-.131100E+03
.191300E+00	-.197500E+03
.256800E+00	-.258800E+03
.320300E+00	-.306600E+03
.379400E+00	-.341200E+03
.434900E+00	-.364700E+03
.484700E+00	-.378200E+03
.529800E+00	-.377000E+03
.570600E+00	-.365400E+03
.586000E+00	-.362500E+03
.639700E+00	-.332000E+03
.697400E+00	-.298700E+03
.757700E+00	-.249100E+03
.821700E+00	-.192900E+03
.884800E+00	-.128300E+03
.948200E+00	-.629000E+02



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION

PLAJ0950.008

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

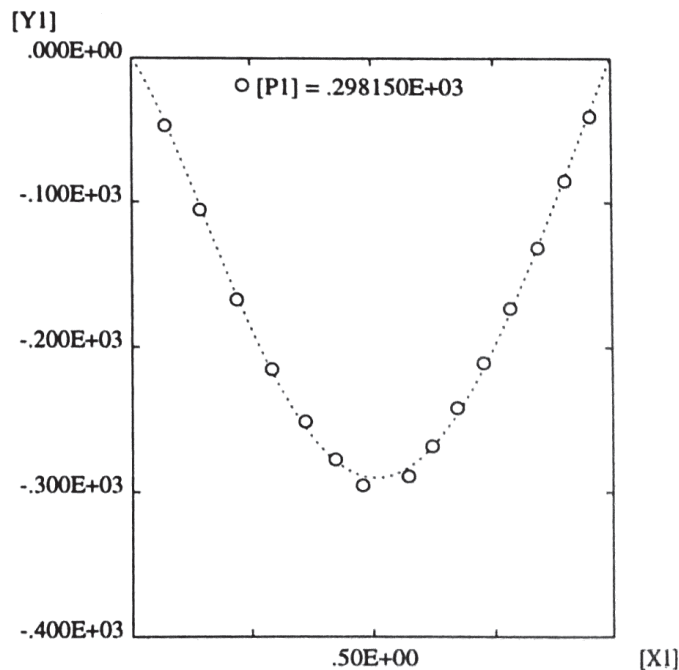
Parameters: [P1] T/K, Temperature

Variables: [X1] x_1 /-, Mole fraction of component 1[Y1] H^E /J mol⁻¹, Molar excess enthalpyMethod: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T

Components: 1. C₂H₂Cl₄, 1,1,2,2-Tetrachloroethane
 2. C₅H₁₁Cl, 1-Chloropentane

[P1] = .298150E+03

[X1]	[Y1]
.707000E-01	-.468000E+02
.144500E+00	-.105400E+03
.221100E+00	-.166600E+03
.293500E+00	-.214600E+03
.361100E+00	-.250600E+03
.422700E+00	-.276600E+03
.478200E+00	-.294700E+03
.572800E+00	-.288300E+03
.620400E+00	-.267900E+03
.672300E+00	-.241500E+03
.726900E+00	-.210100E+03
.784000E+00	-.173000E+03
.841700E+00	-.131000E+03
.899100E+00	-.846000E+02
.954300E+00	-.404000E+02



Property Code: [HMDS1000] HEAT OF MIXING AND SOLUTION

PLAJ0950.009

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

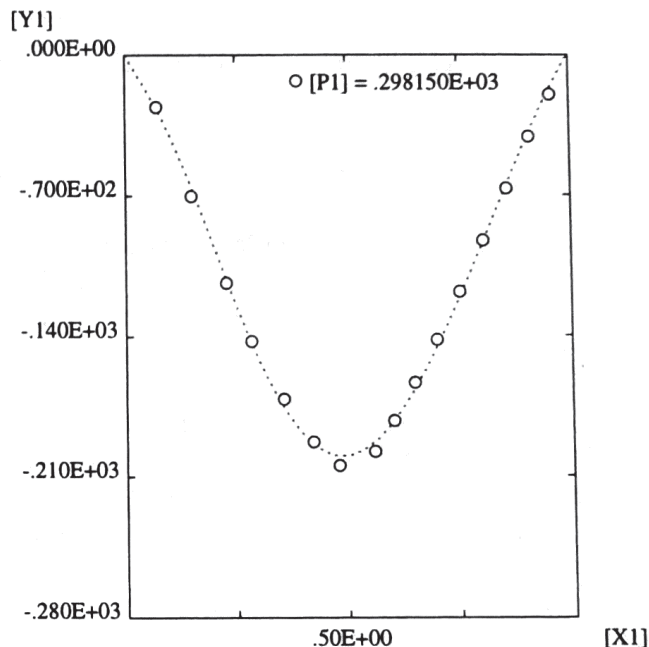
Pure component 1, liquid

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 enthalpyMethod: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T Components: 1. C₂H₂Cl₄, 1,1,2,2-Tetrachloroethane
2. C₆H₁₃Cl, 1-Chlorohexane

[P1] = .298150E+03	
[X1]	[Y1]
.732000E-01	-.259000E+02
.151200E+00	-.701000E+02
.228500E+00	-.113100E+03
.284900E+00	-.142400E+03
.356700E+00	-.171300E+03
.422000E+00	-.192700E+03
.480400E+00	-.204500E+03
.560500E+00	-.197500E+03
.604300E+00	-.182300E+03
.651100E+00	-.163400E+03
.700900E+00	-.141900E+03
.753000E+00	-.118100E+03
.806000E+00	-.926000E+02
.859000E+00	-.666000E+02
.910900E+00	-.409000E+02
.958500E+00	-.196000E+02



Property Code: [HMDS1000] HEAT OF MIXING AND SOLUTION

PLAJ0950.010

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

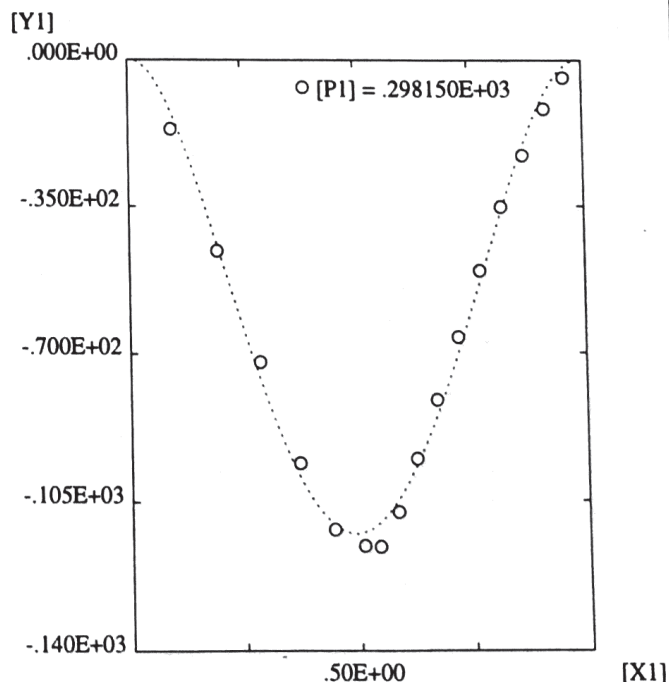
Pure component 1, liquid

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 enthalpyMethod: Direct low-pressure calorimetric measurement of H^E at variable x_1 and constant T Components: 1. C₂H₂Cl₄, 1,1,2,2-Tetrachloroethane
2. C₇H₁₅Cl, 1-Chloroheptane

[P1] = .298150E+03	
[X1]	[Y1]
.966000E-01	-.165000E+02
.194800E+00	-.454000E+02
.286600E+00	-.719000E+02
.370400E+00	-.956000E+02
.444600E+00	-.111400E+03
.509900E+00	-.115300E+03
.544100E+00	-.115600E+03
.584500E+00	-.107400E+03
.627400E+00	-.948000E+02
.673100E+00	-.808000E+02
.721000E+00	-.659000E+02
.770500E+00	-.502000E+02
.819900E+00	-.351000E+02
.869700E+00	-.228000E+02
.918500E+00	-.116000E+02
.962400E+00	-.410000E+01



Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION		PLAJ0950.011	
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 ₂ H ₂ Cl ₄ , 1,1,2,2-Tetrachloroethane 2. C ₈ H ₁₇ Cl, 1-Chlorooctane			
[P1] = .298150E+03			
[X1]	[Y1]		
.886000E-01	-.128000E+02		
.179200E+00	-.199000E+02		
.277300E+00	-.281000E+02		
.355700E+00	-.325000E+02		
.425400E+00	-.353000E+02		
.487500E+00	-.363000E+02		
.548100E+00	-.327000E+02		
.588200E+00	-.195000E+02		
.631000E+00	-.730000E+01		
.676200E+00	.220000E+01		
.723500E+00	.144000E+02		
.772300E+00	.205000E+02		
.822000E+00	.237000E+02		
.870900E+00	.238000E+02		
.919200E+00	.184000E+02		
.962100E+00	.104000E+02		

Property Code: [HMSD1000] HEAT OF MIXING AND SOLUTION		PLAJ0950.012	
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 ₂ H ₂ Cl ₄ , 1,1,2,2-Tetrachloroethane 2. C ₉ H ₁₉ Cl, 1-Chlorononane			
[P1] = .298150E+03			
[X1]	[Y1]		
.981000E-01	.142000E+02		
.193100E+00	.294000E+02		
.285600E+00	.437000E+02		
.369000E+00	.548000E+02		
.443500E+00	.619000E+02		
.508000E+00	.664000E+02		
.564300E+00	.785000E+02		
.612600E+00	.820000E+02		
.670200E+00	.865000E+02		
.711600E+00	.906000E+02		
.755600E+00	.925000E+02		
.800500E+00	.919000E+02		
.844900E+00	.852000E+02		
.888600E+00	.727000E+02		
.930300E+00	.543000E+02		
.967800E+00	.315000E+02		