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Data Article

Behaviour of dichloromethane in solution with hydrocarbons and esters using a database with properties generated in the mixing processes

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ABSTRACT

This work studies the behaviour of a set of binary systems formed by dichloromethane, as the common compound, with six alkanes with an even number of carbon atoms (from hexane to hexadecane), as well as twenty-three alkyl (methyl to pentyl) alkanoates (methanoate to pentanoate). The energetic/volumetric effects produced by the mixing processes were determined point-by-point and represented analytically and graphically using a correlation equation that considers the physical nature of the compounds involved in the binary solutions. This study is a part of a working project investigating the behaviour of halogenated compounds with other compounds and, in this case, expanding knowledge of their interactions in solution. The information used, in the form of (x_1, y^E/Jmol^{-1}) with $y^E = h^E$ or pv^E is considered to be original and consists of over 1000 discrete points measured isothermally at $T = 298.15$ K and isobarically at atmospheric pressure of $\sim$ 98 kPa. The information used is of interest and provides significant value to different sectors, both academic and industrial. The impact of the information provided on

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the theoretical modeling of behaviour of compounds in fluid state, both pure and in solution, is especially valued.

Specifications Table

Subject	Engineering & Materials science
Specific subject area	Thermodynamic, Applications in Chemical Engineering Processes, Theoretical Studies and Modelling.
Type of data	Table, graph,
Data collection	Assessment of the energetic/volumetric effects directly/indirectly determined in the mixing processes of twenty-nine binary systems formed by dichloromethane with alkanes and esters.
Data source location	Division of Thermal Engineering and Instrumentation (IDeTIC), University of Las Palmas de Gran Canaria, 35,017-Las Palmas de Gran Canaria, Spain.
Data accessibility	Repository name: Mendeley Data Data identification number: 10.17632/692ctgbrct.1 Direct URL to data: https://data.mendeley.com/datasets/692ctgbrct/1
Related research article	

1. Value of the Data

- In this work, an extensive database is used as part of a research project analyzing the behaviour of halogenated substances in solution with other organic compounds. Binary solutions containing dihalomethanes are of particular interest. This study examines the energetic and volumetric effects that occur in the mixing processes of dichloromethane with alkanes and esters.
- Studies on the behaviour of dihalomethane solutions are scarce in the scientific literature. The contribution presented in this paper is therefore highlighted, as many of the selected solutions have industrial applications that are useful for engineers as well as for scientific studies. Improving our understanding of these solutions is important for the better design of the processes involving them, specifically those related to process engineering. High-quality real data is required for more accurate modeling.
- Dihalomethanes and esters are used in the synthesis of numerous organic substances for use in the agrochemical and pesticide industries, as well as in the production of dyes, waxes, perfumes, solvents, and cleaning products. Dichloromethane, in particular, is used as a degreaser, paint and varnish stripper, cellulose ester solvent, and polyurethane foam agent, among many other applications. Therefore, the information in this study provides significant added value for characterizing operations of diverse nature.
- The useful of the dataset in future theoretical research is also highlighted. As dichloromethane is toxic, it must be disposed of as waste, which requires prior knowledge of its reactivity with other substances. We therefore anticipate that this information will be valuable in the future development of theoretical-practical studies. Mixtures with alkanes provide useful reference information.

2. Background

In the mid-20th century, many studies were conducted in an attempt to develop a universal theory to explain the behaviour of fluids. Science in general, and scientists in particular, share a common goal: to maximize knowledge of real phenomena in order to understand and

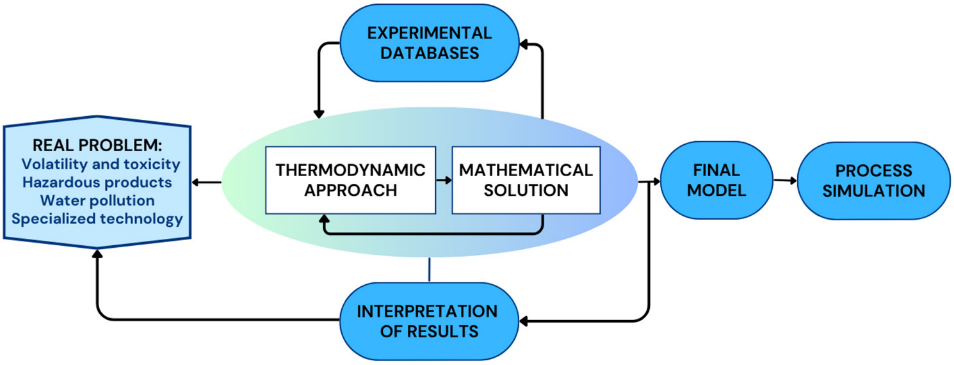

Fig. 1. Scheme showing the sequence of standard actions performed in research tasks.

subsequently control them. One of the main objectives is to understand matter and how it behaves in different situations. Developing a theoretical model to represent fluid matter is one of the challenges of research in this field. However, while scientific development has experienced a significant boom, what can be said about the practical application of these advances? The tasks defined here connect the pure science with practical applications through the development of models or equations that engineers and/or scientists can use. The work presented forms part of a series of actions carried out within the framework of projects that contribute to scientific theory and the practical application of real-world events. The sequence of tasks expressed in both directions, is as follows: experimentation ⇔ theoretical modelling/verification ⇔ simulation/design, as shown in the Fig. 1.

From a theoretical perspective, knowledge of the molecular structure of liquids is essential for verifying and applying a model, as well as for understanding the existing intermolecular and intramolecular forces, i.e. the forces acting between different or identical molecules. The aim of this study is to deepen the understanding of the properties of solutions containing halogenated compounds, a topic that has been the focus of several research teams. Previous work by our group presented experimental and theoretical information on several binary systems containing alkyl halides, and the results were analyzed according to the nature of each compound. Liquid theories were also applied to interpret their behaviour. Consequently, the literature contains numerous publications on various mono-chloroalkanes with alkanes [1,2] and with esters [3,4], di-haloalkanes with alkanes [5] and with esters [6,7], and even with ionic liquids [8], among others. However, few publications show experimental and/or theoretical information on the behaviour of binaries containing a dihalomethane, as one of the components in solution, since the behaviour of these halogenated compounds is unique when they are derivatives of methyl group. This was verified in a previous study [9], which collected experimental data on the behaviour of dibromomethane in solution with alkanes and esters. Specifically, the study reported that the final solutions containing dibromides exhibited expansive volumetric behaviour in all cases, for both hydrocarbons and esters. However, while the h^Es were endothermic in the binaries (dibromomethane + alkane), this was not the case in the (dibromomethane + ester) systems, where the majority exhibited a final exothermic effect $h^E<0$, except for some solutions with methanoates due to the specific interactions of the HCOO/Br-Br pair.

Similarly, there is little information in the literature on the systems with dichloromethane that we are studying. A brief analysis, both quantitative and graphic, of the available information in literature is as follows. Bissel et al. [10] published h^E and v^E data of dichloromethane with hexane and heptane at 298.15 K. With the esters, Van Ness and Abbott [11] determined the h^Es at two temperatures (303.15 and 318.15) K of the same dihalide with methyl ethanoate, as well as v^E at (298.15 and 303.15) K [12]. Avedis et al. [13] published (x, h^E) data of dichloromethane with methyl ethanoate and propanoate, ethyl ethanoate, butyl methanoate at 298.15 K. This information will be used for comparison and to analyse its significance in subsequent operations.

3. Data Description

The densities of thirty pure compounds and twenty-nine binary mixtures, synthesized at different concentrations, formed by dichloromethane as the common compound, with six even-numbered alkanes (from hexane to hexadecane) and twenty-three alkyl (methyl to pentyl) alkanoates (methanoate to pentanoate) were measured directly. Based on the obtained density values, the corresponding volumetric variations generated in the mixing processes were calculated to show the molecular restructuring results of the compounds in the final solution. The numerical information is collected in the Mendeley repository [14], with data of (x_i, $\rho_{i,}$ v^E)∊[0,1] and also of (x_i, h^E)∊[0,1] that were generated in the mixing processes for all the indicated binaries. Fig. 2(a) shows the results of the variation of both magnitudes (x_i,h^E,pv^E) for the binaries x_1 CH_2Cl_2 + x_2 C_nH_{2n+2} (n = 6,8,10,12,14,16) with the hydrocarbon chain n, showing a regular variation of both properties with n and positive energetic effects (endothermic) and expansion effects for all cases, which are qualitatively very similar.

Fig. 2(b) shows the results for the set [x_i, (h^E,pv^E)/Jmol^{-1}] corresponding to the systems with alkyl propanoates. These systems were chosen as examples from among the dichloromethane-ester systems, empirically defined as CH_2Cl_2+$C_2H_5CO_2C_{v\text{-}1}H_{2v+1}$ (v = 1–5). For these mixtures, opposite net enthalpy/volume effects are observed, which we discuss. Our results can be compared with those found in the literature for identical systems. Fig. 3(a) shows a comparison of the curves representing the volumetric effects of the (dichloromethane+C_6) system with those determined by Bissell et al. [10]. Quantitatively, the comparison of the curves for all cases was made with the average absolute relative deviation (% *AARD*) statistic, defined as:

$$\%AARD = \frac{100}{N}\sum_{i=1}^{N}\left[\frac{\left|y^E_{i,cal}(x_1) - y^E_{i,exp}(x_1)\right|}{y^E_{i,exp}(x_1)}\right] \quad (1)$$

where N is the experimental points and y^E the property under study. There are significant differences of more than 40 %, which may be due to the dilatometric measurement technique used by these authors over fifty years ago. However, Fig. 3(b) shows that the enthalpy data for the same system exhibit acceptable differences of around 7.5 %.

In order to understand the behaviour of both dihalomethanes in solution, it is important to briefly compare the results obtained for the h^E/v^E properties of the hydrocarbon binaries

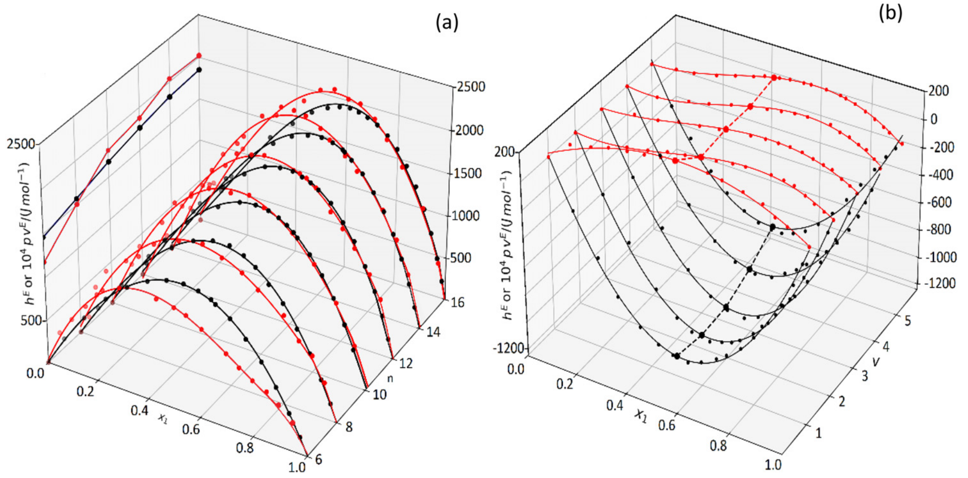

Fig. 2. 3D-plot of energetic quantities h^E (black) and pv^E (red) resulting of mixing process of the binaries: (a) x_1 CH_2Cl_2 + $x_2C_{2n}H_{4n+2}$ (n = 3–8), (b) x_1 CH_2Cl_2 + x_2 $C_2H_5CO_2$ $C_{v\text{-}1}H_{2v+1}$ (v = 1–5).

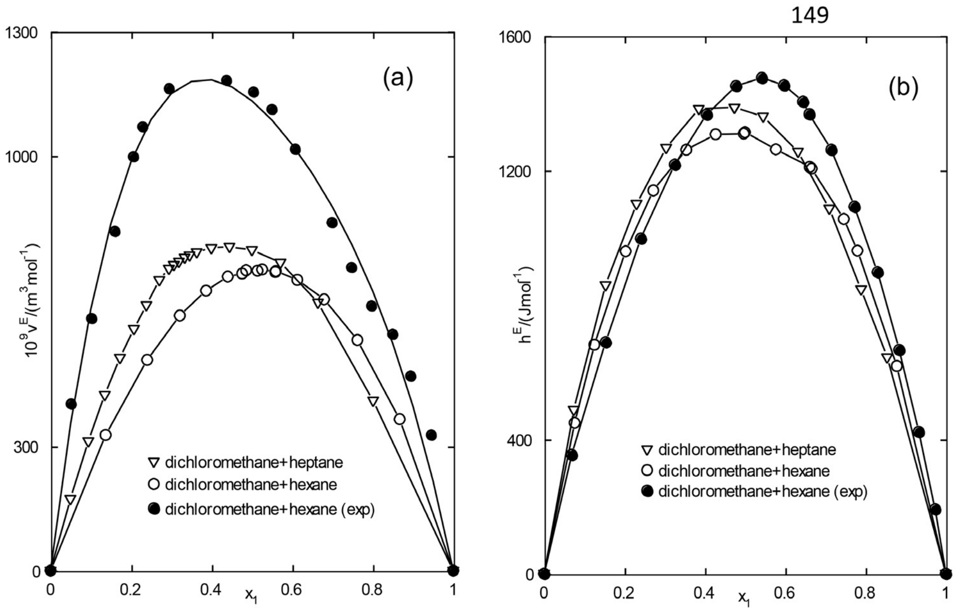

Fig. 3. Comparison between the experimental data used for this work [14] and those from literature, measured at 298.15 K. *AARD* percentage of the compared curves is shown between parentheses for: (a), Excess volumes for: $Cl_2C_2H_2 + C_6$: (●) [14], (○) [10] (> 40 %); (▽) values for $Cl_2C_2H_2 + C_7$ [10]; (b) Excess enthalpies for: $Cl_2C_2H_2 + C_6$: (●) [14], (○) [10] (> 7 %); (▽) values for $Cl_2C_2H_2 + C_7$ [10].

with Br_2CH_2 [9] and those of Cl_2CH_2 in this study. The h^E values measured for systems (dibromomethane + an alkane) are quantitatively higher than those obtained for the corresponding systems with dichloromethane, while the v^E values are higher in binary mixtures containing dichloromethane. This seems logical because the Br atoms are larger than Cl atoms, facilitating better volumetric coupling of the molecules in the final solution, thereby decreasing the v^E values. The mixing processes in these systems are all endothermic $h^E > 0$, and the effects of the binaries with dibromomethane are greater (for the same hydrocarbon), since the overall surface of CH_2Br_2 is much greater than that of CH_2Cl_2, making it easier to polarise and proportionally facilitating the breaking of the halogen-C bond. This results in high values of $h^E \sim 2000$ $Jmol^{-1}$. The corresponding systems with CH_2Cl_2 did not reach this value.

On the other hand, the mixing effects of CH_2Cl_2 binaries with esters did not show such regular variation according to the acidic (u) or alcoholic (v) chain of the ester, $C_{u\text{-}1}H_{2u\text{-}1}$ $CO_2C_vH_{2v+1}$ ($u = 1$–5, $v = 1$–5). A comparative analysis of our values and those of the literature yields the following comments. Fig. 4(a) compares the v^E values at 298.15 K with those determined by Van Ness and Abbott [12]. The values coincide in ester-rich zones; however, our values present a small volume contraction at low concentrations, which seems logical given the low presence of CH_2Cl_2 in an ester-rich solution, with $h^E < 0$. Fig. 4(b) shows the comparison of the enthalpies of four different systems. Generally, our values are higher than those of Avedis et al. [13], and closer to those determined by Van Ness and Abbott [11]. There is no specific explanation to justify these differences, given that the equipment used more than thirty years ago is no longer in use.

The interactions of polar-polar compounds are more complex here. The enthalpic effects are exothermic ($h^E < 0$) in all cases due to specific interactions. The working energies corresponding to molecular rearrangement produce small quantitative volumetric effects, see Fig. 2(b), with the net values resulting from the sum of two particular effects: one of expansion, $v^E > 0$, due to interstitial accommodation and a smaller negative effect, $v^E < 0$ due to the ester-dichloromethane

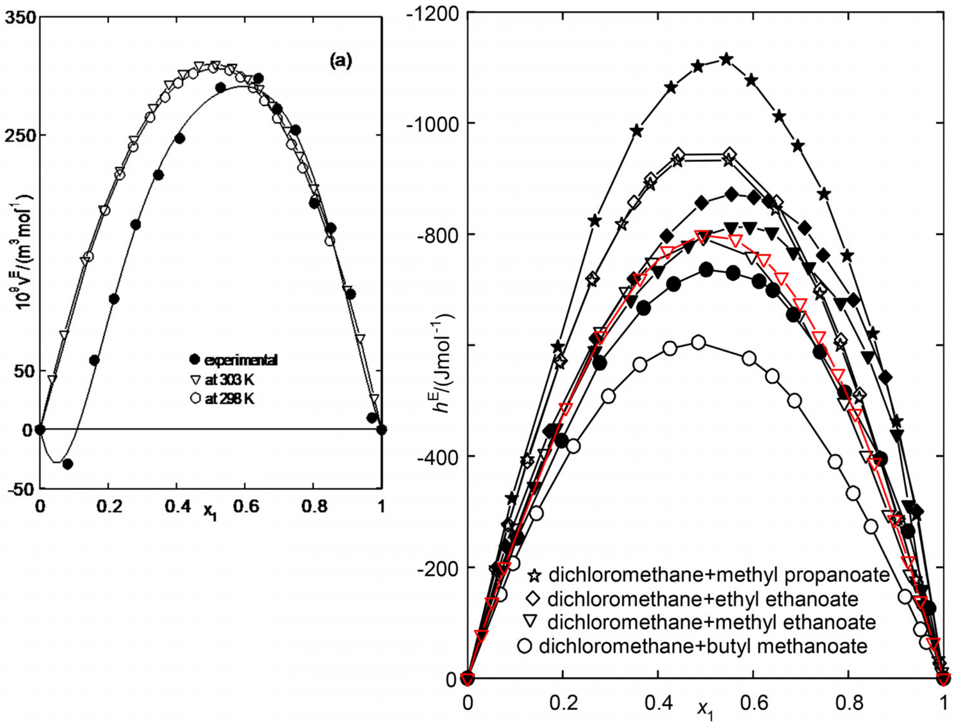

Fig. 4. Comparison between the experimental values used for this work [14] and those from literature measured at 298.15 K. *AARD* percentage of the compared curves is shown between parentheses for: (a) v^E for x_1 Cl_2CH_2 + x_2 $CH_3CO_2CH_3$: (●) [14], (○) [12] (> 70 %); (b) h^E for the same system, empty symbols [11,13], solid symbols [14], ∇ values from ref [11] for x_1 Cl_2CH_2 + x_2 $CH_3CO_2CH_3$ at 303.15 K. (*AARD*) between our curves [14] and those from literature [13], (○,●) (> 25 %); (∇,▼) (>11 %); (♦,◇) (>11 %): (✯,★) (> 17 %).

intermolecular interaction. For these reasons, dichloromethane + ester systems do not exhibit a regular variation with the chain of the ester involved in the mixture, unlike hydrocarbons systems, whose variation is regular (as is logical) with the number of the methyl group $-CH_2-$ of the alkane, see Fig. 2(a).

4. Experimental Design, Materials, and Methods

4.1. Materials

Table 1 shows the list of compounds used in this study, indicating the origin and commercial purity of each compound. Before use, the compounds were subjected to ultrasonic degassing for several hours and then stored in the dark for several days with 0.3 nm Fluka molecular sieve in order to reduce the moisture content. Prior to the experiments, the quality of the products was checked by gas chromatography on an Agilent 4890 N GC, yielding results that were slightly better than those provided by the manufacturer. The quality of the products was also checked by measuring their density ρ and refractive index n_D at 298.15 K and atmospheric pressure. These are shown in Table 2 and were compared with data from the literature [15–21], confirming that they met the appropriate quality standards. As an exception, no n_D data were found for pentyl butanoate. In general, the agreement is acceptable.

Table 1
Commercial specifications of the pure products.

Compound		CAS	Molecular formula	Molecular weight	Supplier	Commercial Purity w/w, %
dichloromethane		75–09–2	Cl_2CH_2	84.932	Merck	>99.5
methyl methanoate	1	107–31–3	$C_2H_4O_2$	60.053	Aldrich	>98.5
methyl ethanoate	2	79–20–9	$C_3H_6O_2$	74.079	Fluka	>99.0
methyl propanoate	3	554–12–1	$C_4H_8O_2$	88.106	Fluka	>99.5
methyl butanoate	4	623–42–7	$C_5H_{10}O_2$	102.133	Fluka	>99.0
methyl pentanoate	5	624–24–8	$C_6H_{12}O_2$	116.160	Fluka	>99.0
ethyl methanoate	6	109–94–4	$C_3H_6O_2$	74.079	Fluka	99.0
ethyl ethanoate	7	141–78–6	$C_4H_8O_2$	88.106	Aldrich	>97.0
ethyl propanoate	8	105–37–3	$C_5H_{10}O_2$	102.133	Fluka	>99.5
ethyl butanoate	9	105–54–4	$C_6H_{12}O_2$	116.160	Fluka	>99.0
ethyl pentanoate	10	539–82–2	$C_7H_{14}O_2$	130.187	Fluka	>98.0
propyl methanoate	11	110–74–7	$C_4H_8O_2$	88.106	Aldrich	99.0
propyl ethanoate	12	109–60–4	$C_5H_{10}O_2$	102.133	Aldrich	>97.0
propyl propanoate	13	106–36–5	$C_6H_{12}O_2$	116.160	Aldrich	99.0
propyl butanoate	14	105–66–8	$C_7H_{14}O_2$	130.187	Fluka	>99.0
butyl methanoate	15	592–84–7	$C_5H_{10}O_2$	102.133	Aldrich	>97.0
butyl ethanoate	16	123–86–4	$C_6H_{12}O_2$	116.160	Aldrich	>97.0
butyl propanoate	17	590–01–2	$C_7H_{14}O_2$	130.187	Fluka	>98.5
butyl butanoate	18	109–21–7	$C_8H_{16}O_2$	144.214	Aldrich	99.0
pentyl methanoate	19	638–49–3	$C_6H_{12}O_2$	116.160	Aldrich	>96.0
pentyl ethanoate	20	628–63–7	$C_7H_{14}O_2$	130.187	Aldrich	>96.0
pentyl propanoate	21	624–54–4	$C_8H_{16}O_2$	144.214	Supelco	>98.0
pentyl butanoate	22	540–18–1	$C_9H_{18}O_2$	158.241	Aldrich	>99.0
pentyl pentanoate	23	2173–56–0	$C_{10}H_{20}O_2$	172.268	Merck	>97.0
hexane	24	110–54–3	C_6H_{14}	86.177	Supelco	>99.0
octane	25	111–65–9	C_8H_{18}	114.231	Aldrich	99.0
decane	26	124–18–5	$C_{10}H_{22}$	142.285	Aldrich	>99.0
dodecane	27	112–40–3	$C_{12}H_{26}$	170.338	Aldrich	>99.0
tetradecane	28	629–59–4	$C_{14}H_{30}$	198.392	Aldrich	>99.0
hexadecane	29	544–76–3	$C_{16}H_{34}$	226.446	Aldrich	>99.0

4.2. Equipment and procedures

The energy generated in the mixing processes is thermodynamically distributed into two terms. One is measured directly due to the net effects produced by the molecular interaction between dichloromethane molecules and the second compounds (alkanes or esters) in the binary mixtures. Another effect, which cannot be measured directly, corresponds to the work or energy of the intermolecular rearrangement in the final solution, evaluated by the change in volume. The first of these effects was assessed using the excess enthalpies $h^E/(\mathrm{J\ mol^{-1}})$ and was measured directly in a Setaram Calvet MS80 calorimeter under quasi-constant temperature T=(298.15±0.01) K and pressure $p \sim 98$ kPa conditions. The apparatus was electrically calibrated using a stable power supply and the Joule effect in order to reproduce the thermograms produced in the mixing processes and thus determine the apparatus's impedance. Correct functioning of the systems was checked by reproducing the h^E of pattern mixtures as indicated in a previous work [16]. The h^E measurements have an error margin of less than 1 %, while the uncertainty in the compositions x_i was estimated at $\pm 3\cdot 10^{-4}$ molar fraction units of dihalomethane.

On the other hand, the volumetric effects, reflected in the $v^E/(\mathrm{m^3 \cdot mol^{-1}})$, were calculated from the densities of the pure compounds and mixtures obtained directly in a DMA-58 digital densimeter from an Anton-Paar, with a reading of ± 0.02 kg m^{-3}. These measurements were taken under the same p and T conditions as indicated above. The temperature of the densimeter was kept quasi-constant by circulating water from a Julabo F20 thermostatic bath, resulting in minimal temperature variations of ± 0.02 K. The densimeter used to measure the densities of the pure compounds and binary solutions was previously calibrated using a standard procedure

Table 2
Properties of pure compounds. Densities and refractive indices measured at $T = 298.15$ K and $p \approx 98$ kPa.

Compound	ρ / kg·m^{-3}		n_D		q_i	r_i	k_v
exp.	lit.	exp.	lit.				
dichloromethane	1316.25	1316.78[15]	1.4210	1.4211[15]	1.998	2.256	–
methyl methanoate	966.49	966.40 [15]	1.3415	1.3415[15]	2.036	2.143	0.963
methyl ethanoate	926.45	927.90[15] 927.01[21]	1.3585	1.3589[15] 1.3592[21]	2.576	2.804	1.239
methyl propanoate	911.17	908.59 [16]	1.3740	1.3745[16]	3.116	3.479	1.499
methyl butanoate	892.38	892.52 [16]	1.3860	1.3852[16]	3.656	4.153	1.774
methyl pentanoate	884.73	884.58[16]	1.3950	1.3947[16]	4.196	4.827	2.035
ethyl methanoate	914.17	915.30[[15]	1.3580	1.3575[15]	2.576	2.817	1.256
ethyl ethanoate	894.33	894.55[15] 894.34[21]	1.3692	1.3698[15] 1.3701[21]	3.116	3.479	1.527
ethyl propanoate	884.02	884.00[15] 883.91[21]	1.3815	1.3814[15] 1.3817[21]	3.656	4.153	1.790
ethyl butanoate	873.54	873.94 [15]	1.3895	1.3900[17]	4.196	4.827	2.061
ethyl pentanoate	869.42	868.98 [18]	1.3980	1.3980[18]	4.736	5.502	2.321
propyl methanoate	899.81	899.60[15]	1.3745	1.3750[15]	3.116	3.492	1.517
propyl ethanoate	882.08	882.60 [15]	1.3815	1.3828[15]	3.656	4.153	1.794
propyl propanoate	875.61	876.70 [17]	1.3900	1.3920[17]	4.196	4.827	2.056
propyl butanoate	876.90	868.20 [17]	1.3970	1.3976[17]	4.736	5.502	2.325
butyl methanoate	888.47	886.90 [15]	1.3870	1.3874[15]	3.656	4.166	1.781
butyl ethanoate	876.48	876.36 [15] 875.62[21]	1.3915	1.3918[15] 1.3921[21]	4.196	4.827	2.054
butyl propanoate	871.08	871.40 [17]	1.3980	1.3989[18]	4.736	5.502	2.316
butyl butanoate	864.84	864.67 [18]	1.4040	1.4040[18]	5.276	6.176	2.584
pentyl methanoate	882.27	891.90 [17]	1.3970	1.3977[17]	4.196	4.841	2.040
pentyl ethanoate	871.86	871.90 [15]	1.4002	1.4000[19]	4.736	5.502	2.314
pentyl propanoate	867.93	867.80 [19]	1.4052	1.4053[19]	5.276	6.176	2.575
pentyl butanoate	862.44	863.0 [20]	1.4102	–	5.816	6.850	2.843
pentyl pentanoate	861.16	860.64 [19]	1.4144	1.4146[19]	6.356	7.524	3.100
hexane	654.81	654.84 [15] 654.82[21]	1.3723	1.3723[15] 1.7375 [21]	3.856	4.500	2.039
octane	698.71	698.62 [15] 698.44[21]	1.3951	1.3951[15] 1.3955 [21]	4.936	5.849	2.534
decane	726.18	726.35 [15] 726.64[21]	1.4098	1.4097[15] 1.4100 [21]	6.016	7.197	3.036
dodecane	745.05	745.18 [15] 745.32[21]	1.4196	1.4195[15] 1.4199 [21]	7.096	8.546	3.543
tetradecane	759.11	759.20 [15]	1.4271	1.4263[15]	8.176	9.895	4.050
hexadecane	769.87	769.94 [17]	1.4325	1.4325[17]	9.256	11.244	4.558

in our laboratory [18,19] with water and nonane. The v^E data obtained showed a cumulative uncertainty of v^E $\pm 2\cdot 10^{-9}$ m^3·mol^{-1}, while the resulting uncertainty in the solution composition is $x \pm 0.0002$. The same thermostatic bath was used to control the temperature of the refractive indices n_D shown in Table 2, in order to verify the purity of the pure compounds. The equipment used was a Abbe type refractometer, Zuzi-320, with a reading error of $n_D \pm 0.0002$ units. It was calibrated using double-distilled water at the working temperature.

The experimental data of both properties $\{x_i,\ y^E(x_i){=}v^E(x_i) \vee y^E(x_i){=}h^E(x_i)\}$ were correlated with a polynomial equation used by us [5–8,18,19] whose expression is:

$$y^E = z_i(1-z_i)\left[y_0 + y_1 z_i + y_2 z_i^2\right]$$

being

$$z_i = \frac{x_i}{\sum_{j=1}^{n} \left(\varsigma_j/\varsigma_i\right) x_j} = \frac{x_i}{x_i + \sum_{j\neq i}^{n} k_{ji} x_j} \qquad (2)$$

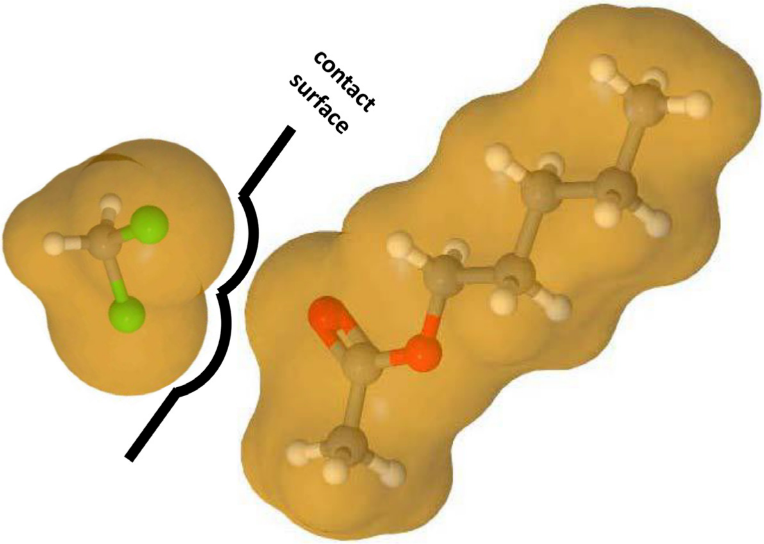

Fig. 5. Plot representing the van der Waals surfaces of dichloromethane and pentyl acetate, as well as the virtual contact surface between them.

The volume change effects are assigned solely to interactions of a physical and/or volumetric nature. Thus, the coefficients ζ_i are identified with the molar volume of substance i that participates in the dissolution. Parameter k_{ji} is therefore the volume ratio of the compounds in the binary, expressed as follows:

$$k_v = \frac{V_2^o}{V_1^o} = \frac{M_2}{M_1}\left(\frac{\rho_1}{\rho_2}\right) \tag{3}$$

where ρ_i and Mi are, respectively, the densities and molecular weight of i. The correlation of the volumes was carried out with Eq. (2) using a non-linear regression method proposed by Nelder-Mead and modified by Lagarias et al. [22], with the value of k_v kept fixed. The values for each binary are shown in Table 2 and have been assigned to the second component of the binary solution. The optimal values of the coefficients y_i of Eq. (2) were obtained for each system by minimizing the following objective function *OF*.

$$OF = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[y_{i,cal}^{E}(x_1) - y_{i,exp}^{E}(x_1)\right]^2} \tag{4}$$

The same *OF* was used to correlate the enthalpy data. In this case, the k_{ji} parameter was identified as k_h and associated with a ratio of interaction surfaces. This is based on the idea that the interaction energies are proportional to the molecular surfaces facing each other of the substances involved in the mixture. This comment results from a global evaluation based on van der Waals-type interactions, which are determined by contact surfaces, see Fig. 5, between portions of both the starting materials (pure components) and the end materials (in the mixture), as well as the polar interactions between polar-polar compounds. Thus, the k_{ji} parameter values correspond either to the volume ratios V_i or the contact areas A_i, as shown in Fig. 5 for the binary formed by dichloromethane (1) and pentyl acetate (2), whose respective areas are A_1=4.95·10^{-9} cm^2/mol and A_2=11.84·10^{-9} cm^2/mol. The area ratio gives rise to the parameter k_h, which can also be calculated using the following expression, as demonstrated by the authors [23].

$$k_h = \left(\frac{q_1}{q_2}\right)\left(\frac{r_2}{r_1}\right)^{2/3} k_v^{2/3} \tag{5}$$

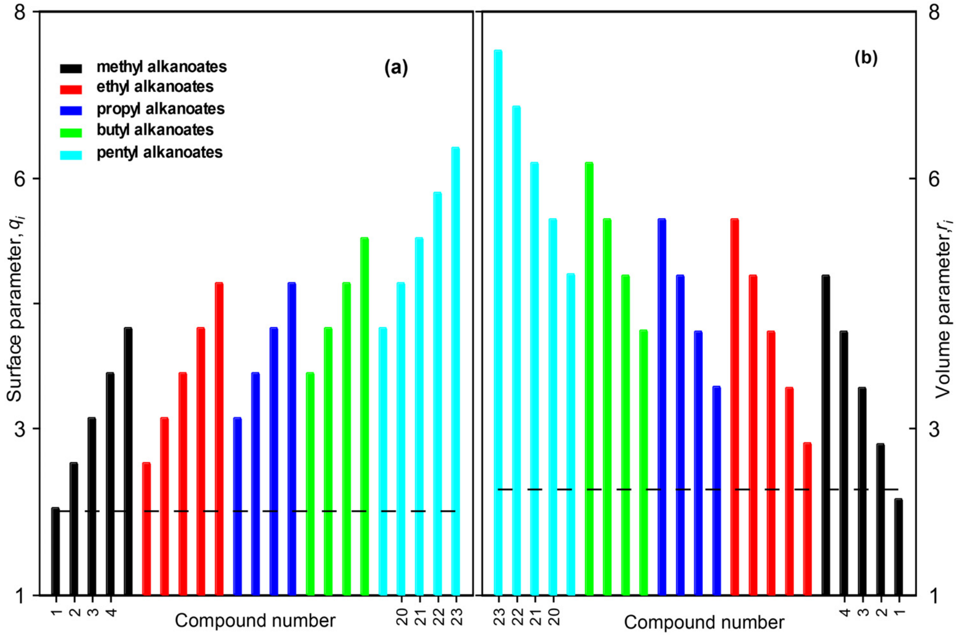

Fig. 6. Bar-chart quantifying the surface area (a) and volume (b) parameters of the esters involved in this study. The dashed-line shows the corresponding values for dichloromethane.

The numerical values of the areas A_i, as well as their corresponding surface q_i and volume r_i parameters, are calculated for each compound using the additive group contribution procedure suggested by Bondi [24]. The numerical values are shown in Table 2. The values of the pairs $[x_i, h^E(x_i)]$ were fitted using the same correlation procedure indicated above, and the resulting curves are shown in Figs. 2–4 of this work.

Fig. 6 (a and b) shows a bar-chart that enables analysis of the differences in the surface parameters q_i and volume r_i between the alkyl alkanoates involved in the twenty-three binaries in this study and dichloromethane. In a similar representation for dihalomethane - an alkane systems, it is easy to image that the differences would correspond to the values of the properties produced by intermolecular interactions, mainly due to van der Waals physical forces. This is especially evident in the case of volumes, where the difference refers to the empty spaces produced by dihalomethane - alkane intermolecular interactions. However, this is not evident in dihalomethane-ester binaries, where act several internal forces act, some of coulombic nature due to the presence of chlorine ions and others purely van der Waals physical forces of different nature (dipolar, dispersive, etc.), which give rise to specific interactions with exothermic processes.

Limitations

None.

Ethics Statement

The authors have read and follow the ethical requirements for publication in Data in Brief and they confirm that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

CRediT Author Statement

Juan Ortega: Conceptualization, Methodology, Validation, Investigation, Writing - Review & Editing, Visualization, Supervision, Project administration, Funding acquisition; **Natalia Cobo:** Writing-Original Draft, Resources; **Mustapha Maarouf:** Data Curation, Formal analysis, Resources, Writing-Review & Editing; **Beatriz Lorenzo:** Data Curation

Data Availability

Mixing properties of binaries {dichloromethane+an alkyl (methyl to pentyl) alkanoate (methanoate to pentanoate), or +an alkane (hexane to hexadecane)} (Original data) (Mendeley Data).

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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