Figure Captions

**Figure 1** – Vapor pressure of methyl esters: (A) L: laurate (☐, Rose and Supina [36]; ◆, Scott et al., [37]); M: myristate (▲, Rose and Supina [36]; ●, Chen et al. [39]); P: palmitate (▲, Hou et al. [40]; ☒, Rose and Supina [36]; ◆, Chen et al. [39]; ◆, Widgren and Bruno [46]); (B) S: stearate (▲, Hou et al. [40]; ☒, Rose and Supina [36]; ◆, Widgren and Bruno [46]); Oa: oleate (▲, Rose and Schrodt [41]; ◆, Scott et al. [37]); La: linoleate (☐, Scott et al. [37]) and Ln: linolenate (○, Scott et al. [37]). Symbols are experimental and lines were calculated using the PC-SAFT model.

**Figure 2** – Vapor pressure curves of ethyl esters: (A) L: laurate (△, Shigley et al. [44]; ☐, Silva et al. [43]); M: myristate (○, Silva et al. [43]; ◆, Tang et al. [45]); P: palmitate (○, Tang et al. [45]); ▲, Silva et al. [43]; ◆, Widgren and Bruno [46]; ●, Silva et al. [53]); (B) S: stearate (▲, Silva et al. [43]; ○ Shigley et al. [44]; ■, Widgren and Bruno [46]); Oa: oleate (☐, Silva et al. [43]; ◆, Ledanos [47]; ▲ Silva et al. [53]) and La: linoleate (■, Silva et al. [43]). Symbols are experimental and lines were calculated using the PC-SAFT model.

**Figure 3** – Density profile as a function of temperature for (A) methyl esters and (B) ethyl esters (L: laurate; M: myristate; P: palmitate; S: stearate; Oa: oleate; La: linoleate and Ln: linolenate (with 1, 2 and 3 double bonds, respectively). Experimental [48] PC-SAFT calculations.

**Figure 4** – Temperatures-composition diagrams for the ethyl esters binary mixtures. (A) ethyl myristate + ethyl palmitate (○, 1.5 kPa; ☐, 1.0 kPa; △, 0.5 kPa [45]), , (B) ethyl palmitate + ethyl oleate (○, 5.3329 kPa; ☐, 9.3326 kPa [53]). Lines are representing predicted values ($k_{ij} = 0$) using both models (—, PC-SAFT; ----, PC-SAFT-JC).

**Figure 5** – Temperatures-composition diagrams for the methyl esters binary mixtures. (A) methyl laurate + methyl myristate (○, 4.0 kPa; ☐, 6.67 kPa; △, 13.33 kPa [36]), (B) methyl myristate + methyl palmitate (○, 1.4 kPa; ☐, 1.0 kPa; △, 0.5 kPa [39]). Lines are representing predicted values ($k_{ij} = 0$) using both models (—, PC-SAFT; ----, PC-SAFT-JC).

**Figure 6** – Temperatures-composition diagrams for the methyl palmitate(1) + methyl stearate(2) system. Symbols are experimental data at different pressures (☐, 0.5333 kPa [54]; ○, 3.947 kPa [36]; ◆, 10.0 kPa; ■, 5.0 kPa; ●, 1.0 kPa and ▲, 0.1 kPa [40]). Lines are the calculated values using both models (—, PC-SAFT; ----, PC-SAFT-JC) with $k_{ij} = 0$ (A) and $k_{ij} = 0.01$ (B).
**Figure 7** – Experimental and predicted melting points for ethyl esters: (A) (Δ, ethyl oleate(1) + ethyl laurate(2); □, ethyl palmitate(1) + ethyl laurate(2)) and (B) (●, ethyl linoleate(1) + ethyl palmitate(2); ○, ethyl oleate(1) + ethyl palmitate(2)). Calculated lines are the PC-SAFT model ($k_{ij} = 0$).

**Figure 8** – VLE diagram for the systems ethanol(1) + hexyl acetate(2) and methanol(1) + hexyl acetate(2). Symbol are experimental data [58] and lines the PC-SAFT model using transferable cross-association parameters ($k_{ij} = 0$).

**Figure 9** – Temperature-composition diagram for the systems (A) ethanol(1)+ethyl palmitate(2) and (B) ethanol(1)+ethyl stearate (2). Symbol are experimental data (Δ, 24 kPa; ○, 92 kPa [7]) and lines the PC-SAFT model using transferable cross-association parameters (—, PC-SAFT; ·····, PC-SAFT-JC) with $k_{ij} = 0$.

**Figure 10** – Pressure-composition diagram for the systems (A) ethanol(1) + ethyl laurate(2), (B) ethanol(1) + ethyl myristate(2), (C) methanol(1) + methyl laurate(2) and (D) methanol(1) + methyl myristate(2), at high temperatures. Symbol are experimental data (Δ, 493 K; □, 523 K; ○, 543 K, [60,61]) and lines are the calculated values using transferable cross-association parameters (—, PC-SAFT; ·····, PC-SAFT-JC) with $k_{ij} = 0$. 
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Figure 10