Data Article

Data supporting the prediction of the properties of eutectic organic phase change materials

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ABSTRACT

The data presented in this article include the molar masses, melting temperatures, latent heats of fusion and temperature-dependent heat capacities of fifteen fatty acid phase change materials (PCMs). The data are used in conjunction with the thermodynamic models discussed in Kahwaji and White (2018) [1] to develop a computational tool that calculates the eutectic compositions and thermal properties of eutectic mixtures of PCMs. The computational tool is part of this article and consists of a Microsoft Excel® file available in Mendeley Data repository [2]. A description of the computational tool along with the properties of nearly 100 binary mixtures of fatty acid PCMs calculated using this tool are also included in the present article. The Excel® file is designed such that it can be easily modified or expanded by users to calculate the properties of eutectic mixtures of other classes of PCMs.

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The data presented in this article include the molar masses and thermal properties of 15 fatty acid PCMs (Table 1). The thermal properties are the melting temperature, \( T_{\text{mpt}} \), the latent heat of fusion, \( \Delta_{\text{fus}}H \), and the heat capacities, \( C_p(T) \), of both the solid and liquid phases. We measured \( T_{\text{mpt}}, \Delta_{\text{fus}}H \) and \( C_p(T) \) of five fatty acids: decanoic acid (C10 thereafter), dodecanoic acid (C12), tetradecanoic acid (C14), hexadecanoic acid (C16) and octadecanoic acid (C18) by DSC [3], whereas for the other fatty acids, the values of \( T_{\text{mpt}}, \Delta_{\text{fus}}H \) and \( C_p(T) \) were obtained from the literature [4,5]. The data in Table 1 are the basis of the Excel® file, available from [2]. The Excel® file contains equations from the thermodynamic models discussed in the manuscript entitled “Prediction of the Properties of Eutectic Fatty Acid Phase Change Materials” [1] and was used to compute the eutectic compositions and thermal properties of all 105 possible binary combinations of the fatty acid PCMs. A total of 97 combinations form binary eutectic mixtures and their properties are included in Tables 2–5, presented according to the range of the eutectic temperature, \( T_{\text{eut}} \), of the mixtures.
Table 1
Thermal properties of fatty acid PCMs. The properties shown in bold were measured in our previous work [4] whereas \( T_{\text{mpt}} \) and \( \Delta_{\text{mix}} H \) of other PCMs are from [5] and references therein. The heat capacities \( C_{p,s}(T) \) and \( C_{p,l}(T) \) of the measured samples (in bold) were obtained from polynomial functions fit close to the transition point, whereas the other \( C_{p,s}(T) \) and \( C_{p,l}(T) \) are from Ref. [6], obtained from wider temperature ranges.

| PCMs                        | Molar mass (g mol\(^{-1}\)) | \( T_{\text{mpt}} \) (°C) | \( \Delta_{\text{mix}} H \) (J g\(^{-1}\)) | \( C_{p,s}(T) \) | \( C_{p,l}(T) \) |
|-----------------------------|------------------------------|-----------------------------|-------------------------------------------|-----------------|-----------------|
| Heptanoic (enanthic) acid   | 130.18                       | 7.4                         | 107                                       | 164.213 – 1.19T + 6.15 \times 10^{-3} T^2 | 72.739 + 1.36T – 3.30 \times 10^{-3} T^2 + 3.33 \times 10^{-6} T^3 |
| Nonanoic (pelargonic) acid  | 156.24                       | 12.3                        | 127                                       | 19 + 1.4T       | 184.223 + 1.21T – 2.92 \times 10^{-3} T^2 + 3.22 \times 10^{-6} T^3 |
| Oleic (elanic) acid         | 282.47                       | 13.5                        | 140                                       | 77.434 + 1.66T  | 278.686 + 2.54T – 5.44 \times 10^{-3} T^2 + 4.92 \times 10^{-6} T^3 |
| Octanoic (caprylic) acid    | 144.21                       | 16.5                        | 148                                       | 241.472 – 1.61T + 6.49 \times 10^{-3} T^2 | 184.525 + 9.97 \times 10^{-3} T – 2.42 \times 10^{-3} T^2 + 2.70 \times 10^{-6} T^3 |
| Undecanoic (undecylic) acid | 186.29                       | 28.4                        | 139                                       | 11 + 1.46T      | 73.094 + 2.34T – 5.29 \times 10^{-3} T^2 + 4.80 \times 10^{-6} T^3 |
| **Decanoic (capric) acid**  | **172.26**                   | **32.0**                    | **145**                                   | **4694.26 – 33.20 T + 6.28 \times 10^{-2} T^2** | **37041.70 – 335.91 T + 1.023 T^2 – 1.04 \times 10^{-3} T^3** |
| Tridecanoic (tridecylic) acid | 214.34                      | 41.8                        | 157                                       | 13 + 1.47T      | 22.393 + 3.05T – 6.67 \times 10^{-3} T^2 + 5.72 \times 10^{-6} T^3 |
| **Dodecanoic (lauric) acid** | **200.32**                   | **43.6**                    | **176**                                   | **4463.56 – 31.40 T + 5.94 \times 10^{-2} T^2** | **208668.96 – 1877.0 T + 5.64 T^2 – 5.65 \times 10^{-3} T^3** |
| Pentadecanoic (pentadecylic) acid | 242.40                     | 52.5                        | 165                                       | 164.349 – 0.283 T + 4.37 \times 10^{-3} T^2 | – 88.671 + 4.08 T – 8.64 \times 10^{-3} T^2 + 7.08 \times 10^{-6} T^3 |
| **Tetradecanoic (myristic) acid** | **228.37**                | **54.7**                    | **186**                                   | **10509.23 – 70.04 T + 1.22 \times 10^{-1} T^2** | **93410.37 – 798.097 T + 2.28 T^2 – 2.17 \times 10^{-3} T^3** |
| Hexadecanoic (palmitic) acid | 256.43                       | 61.7                        | 206                                       | 13440.42 – 87.3 T + 1.47 \times 10^{-1} T^2 | 59987.38 – 491.627 + 1.35 T^2 – 1.24 \times 10^{-3} T^3 |
| Heptadecanoic (heptadecylic) acid | 270.45                     | 62.8                        | 193                                       | 17 + 1.57T      | – 93.243 + 4.467 – 9.20 \times 10^{-3} T^2 + 7.21 \times 10^{-6} T^3 |
| Nonadecanoic (nonadecylic) acid | 298.50                     | 68.0                        | 193                                       | 190.219 – 0.201T + 4.82 \times 10^{-3} T^2 | – 172.759 + 5.25 T – 1.05 \times 10^{-3} T^2 + 7.99 \times 10^{-6} T^3 |
| Octadecanoic (stearic) acid | 284.48                       | 68.4                        | 211                                       | 8670.10 – 55.96 T + 9.62 \times 10^{-3} T^2 | 97806.94 – 7767.7 T + 2.13 T^2 – 1.98 \times 10^{-4} T^3 |
| Eicosanoic (arachidic) acid | 312.53                       | 75.0                        | 227                                       | 20 + 1.77T      | – 169.969 + 5.35 T – 1.06 \times 10^{-2} T^2 + 7.84 \times 10^{-6} T^3 |
Table 2
The eutectic compositions, \( x_{A,E} \), eutectic temperatures, \( T_E \), and eutectic latent heats of fusion \( \Delta_{\text{fus}} H_E \) of binary mixtures of fatty acids calculated using the computational tool described in the text and the data of Table 1. Each eutectic composition is given in terms of the mole fraction of “Component A” and values of \( T_E \) have been rounded to 1°. Data in this table include mixtures with \(-22 < T_E < 0 \) °C.

| Component A                  | Component B                  | \( x_{A,E} \) | \( T_E \) (°C) | \( \Delta_{\text{fus}} H_E \) (kJ mol\(^{-1}\)) |
|------------------------------|------------------------------|---------------|---------------|----------------------------------------|
| Heptanoic (enanthic) acid    | Nonanoic (pelargonic) acid   | 0.685         | −22           | 16.1                                   |
| Heptanoic (enanthic) acid    | Octanoic (caprylic) acid     | 0.725         | −20           | 15.6                                   |
| Heptanoic (enanthic) acid    | Undecanoic (undecylic) acid  | 0.825         | −15           | 16.1                                   |
| Heptanoic (enanthic) acid    | Decanoic (capric) acid       | 0.835         | −15           | 15.5                                   |
| Heptanoic (enanthic) acid    | Oleic (elainic) acid         | 0.835         | −15           | 16.9                                   |
| Heptanoic (enanthic) acid    | Tridecanoic (tridecylic) acid| 0.925         | −11           | 15.3                                   |
| Heptanoic (enanthic) acid    | Dodecanoic (lauric) acid     | 0.935         | −10           | 13.6                                   |
| Heptanoic (enanthic) acid    | Pentadecanoic (pentadeicylic)acid | 0.965     | −9            | 14.7                                   |
| Nonanoic (pelargonic) acid   | Octanoic (caprylic) acid     | 0.545         | −7            | 20.5                                   |
| Nonanoic (pelargonic) acid   | Oleic (elainic) acid         | 0.630         | −3            | 25.8                                   |
| Nonanoic (pelargonic) acid   | Undecanoic (undecylic) acid  | 0.670         | −1            | 22.2                                   |
| Oleic (elainic) acid         | Octanoic (caprylic) acid     | 0.425         | −1            | 27.1                                   |
| Nonanoic (pelargonic) acid   | Decanoic (capric) acid       | 0.685         | 0             | 22.1                                   |

Table 3
The eutectic properties of fatty acid binary mixtures with \( 0 < T_E < 20 \) °C.

| Component A                  | Component B                  | \( x_{A,E} \) | \( T_E \) (°C) | \( \Delta_{\text{fus}} H_E \) (kJ mol\(^{-1}\)) |
|------------------------------|------------------------------|---------------|---------------|----------------------------------------|
| Octanoic (caprylic) acid     | Undecanoic (undecylic) acid  | 0.630         | 2             | 22.9                                   |
| Octanoic (caprylic) acid     | Decanoic (capric) acid       | 0.645         | 3             | 22.9                                   |
| Oleic (elainic) acid         | Undecanoic (undecylic) acid  | 0.585         | 5             | 32.5                                   |
| Oleic (elainic) acid         | Decanoic (capric) acid       | 0.610         | 5             | 33.0                                   |
| Nonanoic (pelargonic) acid   | Tridecanoic (tridecylic) acid| 0.815         | 5             | 22.4                                   |
| Nonanoic (pelargonic) acid   | Dodecanoic (lauric) acid     | 0.835         | 6             | 21.6                                   |
| Octanoic (caprylic) acid     | Tridecanoic (tridecylic) acid| 0.780         | 9             | 23.6                                   |
| Nonanoic (pelargonic) acid   | Pentadecanoic (pentadeicylic)acid | 0.900     | 9             | 21.7                                   |
| oleic (elainic) acid         | Tridecanoic (tridecylic) acid| 0.775         | 9             | 37.0                                   |
| Octanoic (caprylic) acid     | Dodecanoic (lauric) acid     | 0.800         | 9             | 23.3                                   |
| Octanoic (caprylic) acid     | Tetradecanoic (myristic) acid| 0.920         | 9             | 20.8                                   |
| Oleic (elainic) acid         | Dodecanoic (lauric) acid     | 0.800         | 10            | 37.1                                   |
| Undecanoic (undecylic) acid  | Dodecanoic (capric) acid     | 0.525         | 11            | 26.4                                   |
| Nonanoic (pelargonic) acid   | Hexadecanoic (palmitic) acid | 0.965         | 11            | 20.7                                   |
| Nonanoic (pelargonic) acid   | Heptadecanoic (heptadeicylic)acid | 0.965     | 11            | 20.8                                   |
| Oleic (elainic) acid         | Pentadecanoic (pentadeicylic)acid | 0.880     | 11            | 38.7                                   |
| Nonanoic (pelargonic) acid   | Nonadecanoic (nonadeicylic) acid | 0.980     | 12            | 20.5                                   |
| Nonanoic (pelargonic) acid   | Octadecanoic (stearic) acid  | 0.985         | 12            | 20.1                                   |
| Oleic (elainic) acid         | Tetradecanoic (myristic) acid| 0.905         | 12            | 38.4                                   |
| Octanoic (caprylic) acid     | Pentadecanoic (pentadeicylic)acid | 0.875     | 12            | 23.3                                   |
| Oleic (elainic) acid         | Hexadecanoic (palmitic) acid | 0.960         | 13            | 39.5                                   |
| Oleic (elainic) acid         | Heptadecanoic (heptadeicylic)acid | 0.960     | 13            | 39.6                                   |
| Octanoic (caprylic) acid     | Tetradecanoic (myristic) acid| 0.895         | 13            | 22.5                                   |
| Oleic (elainic) acid         | Nonadecanoic (nonadeicylic) acid | 0.980     | 13            | 39.7                                   |
| Oleic (elainic) acid         | Octadecanoic (stearic) acid  | 0.985         | 13            | 39.4                                   |
| Octanoic (caprylic) acid     | Hexadecanoic (palmitic) acid | 0.955         | 15            | 22.3                                   |
| Octanoic (caprylic) acid     | Heptadecanoic (heptadeicylic)acid | 0.955     | 15            | 22.5                                   |
| Octanoic (caprylic) acid     | Nonadecanoic (nonadeicylic) acid | 0.975     | 16            | 22.1                                   |
| Octanoic (caprylic) acid     | Octadecanoic (stearic) acid  | 0.980         | 16            | 21.7                                   |
| Undecanoic (undecylic) acid  | Tridecanoic (tridecylic) acid| 0.665         | 17            | 28.3                                   |
| Undecanoic (undecylic) acid  | Dodecanoic (lauric) acid     | 0.690         | 18            | 29.0                                   |
| Decanoic (capric) acid       | Tridecanoic (tridecylic) acid| 0.640         | 19            | 28.8                                   |
| Decanoic (capric) acid       | Dodecanoic (lauric) acid     | 0.665         | 20            | 29.6                                   |
Table 4
The eutectic properties of fatty acid binary mixtures with $20 < T_E < 40 \degree C$.

| Component A                  | Component B                                  | $x_{AE}$ | $T_E \degree C$ | $\Delta_{fus-H_E} (kJ \text{ mol}^{-1})$ |
|------------------------------|-----------------------------------------------|----------|-----------------|-----------------------------------------|
| Undecanoic (undecylic) acid  | Pentadecanoic (pentadecylic) acid             | 0.790    | 22              | 28.6                                    |
| Undecanoic (undecylic) acid  | Tetradecanoic (myristic) acid                 | 0.815    | 23              | 28.1                                    |
| Decanoic (capric) acid       | Pentadecanoic (pentadecylic) acid             | 0.760    | 24              | 29.0                                    |
| Decanoic (capric) acid       | Tetradecanoic (myristic) acid                 | 0.790    | 25              | 28.5                                    |
| Undecanoic (undecylic) acid  | Hexadecanoic (palmitic) acid                  | 0.900    | 25              | 28.2                                    |
| Undecanoic (undecylic) acid  | Heptadecanoic (heptadecylic) acid             | 0.905    | 26              | 28.0                                    |
| Undecanoic (undecylic) acid  | Nonadecanoic (nonadecylic) acid               | 0.940    | 27              | 27.7                                    |
| Undecanoic (undecylic) acid  | Octadecanoic (stearic) acid                   | 0.945    | 27              | 27.2                                    |
| Tridecanoic (tridecylic) acid| Dodecanoic (lauric) acid                      | 0.525    | 27              | 35.0                                    |
| Undecanoic (undecylic) acid  | Eicosanoic (arachidic) acid                   | 0.980    | 28              | 26.7                                    |
| Decanoic (capric) acid       | Hexadecanoic (palmitic) acid                  | 0.880    | 28              | 28.4                                    |
| Decanoic (capric) acid       | Heptadecanoic (heptadecylic) acid             | 0.885    | 28              | 28.1                                    |
| Decanoic (capric) acid       | Nonadecanoic (nonadecylic) acid               | 0.925    | 30              | 27.6                                    |
| Decanoic (capric) acid       | Octadecanoic (stearic) acid                   | 0.930    | 30              | 27.1                                    |
| Decanoic (capric) acid       | Eicosanoic (arachidic) acid                   | 0.970    | 31              | 26.3                                    |
| Tridecanoic (tridecylic) acid| Dodecanoic (lauric) acid                      | 0.640    | 31              | 35.3                                    |
| Tridecanoic (tridecylic) acid| Tetradecanoic (myristic) acid                 | 0.675    | 32              | 35.7                                    |
| Dodecanoic (lauric) acid     | Pentadecanoic (pentadecylic) acid             | 0.620    | 33              | 37.8                                    |
| Dodecanoic (lauric) acid     | Tetradecanoic (myristic) acid                 | 0.655    | 34              | 38.3                                    |
| Tridecanoic (tridecylic) acid| Hexadecanoic (palmitic) acid                  | 0.790    | 36              | 37.3                                    |
| Tridecanoic (tridecylic) acid| Heptadecanoic (heptadecylic) acid             | 0.795    | 36              | 36.7                                    |
| Dodecanoic (lauric) acid     | Hexadecanoic (palmitic) acid                  | 0.770    | 38              | 40.0                                    |
| Tridecanoic (tridecylic) acid| Nonadecanoic (nonadecylic) acid               | 0.860    | 38              | 36.7                                    |
| Tridecanoic (tridecylic) acid| Octadecanoic (stearic) acid                   | 0.870    | 38              | 36.3                                    |
| Pentadecanoic (pentadecylic) acid | Eicosanoic (arachidic) acid                   | 0.895    | 40              | 40.5                                    |
| Dodecanoic (lauric) acid     | Nonadecanoic (nonadecylic) acid               | 0.840    | 40              | 39.3                                    |
| Dodecanoic (lauric) acid     | Octadecanoic (stearic) acid                   | 0.855    | 40              | 38.9                                    |
| Tridecanoic (tridecylic) acid| Eicosanoic (arachidic) acid                   | 0.935    | 40              | 35.8                                    |

Table 5
The eutectic properties of fatty acid binary mixtures with $40 < T_E < 70 \degree C$.

| Component A                  | Component B                                  | $x_{AE}$ | $T_E \degree C$ | $\Delta_{fus-H_E} (kJ \text{ mol}^{-1})$ |
|------------------------------|-----------------------------------------------|----------|-----------------|-----------------------------------------|
| Dodecanoic (lauric) acid     | Eicosanoic (arachidic) acid                   | 0.925    | 42              | 38.0                                    |
| Pentadecanoic (pentadecylic) acid | Hexadecanoic (palmitic) acid                  | 0.660    | 44              | 44.1                                    |
| Pentadecanoic (pentadecylic) acid | Heptadecanoic (heptadecylic) acid             | 0.670    | 44              | 43.1                                    |
| Tetradecanoic (myristic) acid | Heptadecanoic (heptadecylic) acid             | 0.640    | 46              | 45.3                                    |
| Pentadecanoic (pentadecylic) acid | Nonadecanoic (nonadecylic) acid               | 0.750    | 46              | 43.9                                    |
| Pentadecanoic (pentadecylic) acid | Octadecanoic (stearic) acid                   | 0.765    | 47              | 44.0                                    |
| Tetradecanoic (myristic) acid | Nonadecanoic (nonadecylic) acid               | 0.720    | 48              | 46.5                                    |
| Tetradecanoic (myristic) acid | Octadecanoic (stearic) acid                   | 0.735    | 48              | 46.7                                    |
| Pentadecanoic (pentadecylic) acid | Eicosanoic (arachidic) acid                   | 0.860    | 49              | 43.8                                    |
| Hexadecanoic (palmitic) acid | Heptadecanoic (heptadecylic) acid             | 0.515    | 50              | 52.1                                    |
| Tetradecanoic (myristic) acid | Eicosanoic (arachidic) acid                   | 0.835    | 51              | 46.8                                    |
| Hexadecanoic (palmitic) acid | Nonadecanoic (nonadecylic) acid               | 0.605    | 53              | 54.8                                    |
| Hexadecanoic (palmitic) acid | Octadecanoic (stearic) acid                   | 0.620    | 53              | 55.6                                    |
| Heptadecanoic (heptadecylic) acid | Nonadecanoic (nonadecylic) acid               | 0.590    | 54              | 53.5                                    |
| Heptadecanoic (heptadecylic) acid | Octadecanoic (stearic) acid                   | 0.605    | 54              | 54.4                                    |
| Hexadecanoic (palmitic) acid | Eicosanoic (arachidic) acid                   | 0.745    | 57              | 57.2                                    |
| Nonadecanoic (nonadecylic) acid | Octadecanoic (stearic) acid                   | 0.515    | 57              | 58.4                                    |
| Heptadecanoic (heptadecylic) acid | Eicosanoic (arachidic) acid                   | 0.730    | 57              | 56.3                                    |
| Nonadecanoic (nonadecylic) acid | Eicosanoic (arachidic) acid                   | 0.645    | 61              | 61.6                                    |
| Octadecanoic (stearic) acid | Eicosanoic (arachidic) acid                   | 0.635    | 61              | 63.4                                    |
2. Experimental design, materials and methods

The melting temperatures, $T_{mpt}$, $\Delta_{fus}H$ and $C_p(T)$ of the fatty acids (C10, C12, C14, C16 and C18 (Table 1)) were measured with a TA Instruments Q200 DSC, as described in [3]. Each melting temperature was determined from the onset of the DSC endothermic peak, $T_{onset}$, measured at a rate of 2 K min$^{-1}$, whereas $\Delta_{fus}H$ was averaged from the areas of the melting peaks of five melt-freeze cycles measured at 10 K min$^{-1}$ [3,6]. The measured data were added to data from the literature [4,5] for 10 other fatty acid PCMs and included as a database in the Microsoft Excel® workbook. Equations that model the liquidus transitions of simple eutectic mixtures, and equations that calculate the change in enthalpy from the total change of entropy due to mixing, were also implemented in the workbook. The thermodynamic models from which these equations are derived are described in the research paper related to this data article.

The Excel® workbook serves as a computational tool that predicts the properties of binary eutectic mixtures, once the individual compounds of the mixtures are selected by the user. It is designed so that only basic knowledge of Excel® is needed to use the file or to modify it to compute the eutectic properties of other PCMs. A detailed description of the contents of the workbook and of the calculation procedures are presented here to guide users with the manipulation of this file.

The selection of the binary compounds of the eutectic mixture for which the properties are to be calculated, and the results of the calculations are included in the worksheet “Parameters and Results”. As a first step for the calculations of the eutectic properties, the properties of individual PCMs should be entered in the worksheet “PCM data”. The properties required are: the molar mass (in g mol$^{-1}$), $T_{mpt}$ (°C), $\Delta_{fus}H$ (J g$^{-1}$) and $C_p(T)$ for the solid and liquid phases (J mol$^{-1}$ K$^{-1}$). The temperature-dependent heat capacities are entered as a 2nd degree polynomial for the solid phase, $C_p,s(T)$, and as a 3rd degree polynomial for the liquid phase, $C_p,l(T)$. Once the database is loaded, the user uses the worksheet “Parameters and Results” and selects Component A and Component B from the dropdown lists and the calculated properties are displayed in the highlighted cells. The details of the calculations of the eutectic temperature are included in the worksheet “Calculations”. In this worksheet, the mole fractions of components A and B, $x_A$ and $x_B$, are generated and Eqs. (2) and (3) of Ref. [1] are used to calculate the melting temperatures at each $x_A$ and $x_B$ and establish the two liquidus lines. The corresponding mass fractions, $m_A$ and $m_B$, are also calculated from the molar masses of the two components, $M_A$ and $M_B$. For example, the mass fraction of component A is given by:

$$m_A = x_A \left( \frac{M_A}{x_AM_A + x_BM_B} \right)$$

(1)

When the two liquidus lines are calculated, a formula in the workbook identifies the coordinates of their intersection, that is the composition of the eutectic mixture $x_{A,E}$ and the eutectic temperature, $T_E$. Plots of temperature versus composition ($x_A$ and $m_A$ by default) are also generated in the “Calculations” worksheet.

The values determined for $x_{A,E}$, $x_{B,E}$ and $T_E$ are then used to calculate the changes in entropy, $\Delta S$, and estimate the latent heat of fusion of the eutectic mixture, $\Delta_{fus}H_E$ (Eqs. (5)–(12) in [1]). In these calculations, the coefficients of the 3rd degree function $C_p,s(T)$ and those of the 2nd degree function $C_p,l(T)$ are used. Graphs that compare the calculated values of individual $\Delta S_i$ and $\Delta H_i$ ($i = 1–7$, see Fig. 1 in [1] or the figure in the Excel® file) are also included. The variations $\Delta H_i$ give an idea as to which transition contributes more to the total $\Delta_{fus}H_E$.

As discussed above, the calculations of the eutectic properties are initiated when the user selects the two components of a binary mixture. Conversely, the provided workbook is also designed to allow the user to specify a melting temperature and the computational tool predicts which binary mixtures yield that temperature. In the “Parameters and Results” worksheet, the user inputs the desired melting temperature (cell D3) and the workbook determines the five binary compositions with the closest $T_E$. The composition of each of the five eutectic mixtures $x_{A,E}$, along with $T_E$ and $\Delta_{fus}H_E$ are displayed. However, these predictions require prior calculations of the properties of all possible binary combinations (included in the worksheet “Calculations” in the Excel® file). The modification of this prediction method requires a somewhat more advanced knowledge of Microsoft Excel®.
It is possible to modify the current Excel® workbook by replacing entries in the provided database with other values from the users (e.g., direct measurement or other data sources). This approach is especially recommended when estimating the properties of a eutectic mixture formed from materials that might have different purities, and hence different melting points and latent heats (Kahwaji and White, 2017) [1]. Users also can expand the current database by adding entries for compounds. For example, by adding data for an additional fatty alcohol PCM, the workbook can compute the properties of up to 15 new PCM eutectic mixtures. Moreover, although the current workbook calculates the properties of only binary mixtures, it can be expanded to ternary and higher order mixtures using the calculated properties. This can be done since a ternary mixture, for example, is assumed to be a pseudo-binary mixture consisting of an individual fatty acid and a binary eutectic mixture.

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