

## Review of Low-Cost Organic and Inorganic Phase Change Materials with Phase Change Temperature between 0°C and 65°C

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### ABSTRACT

Phase change materials (PCMs) that undergo a phase transition may be used to provide a nearly isothermal latent heat storage at the phase change temperature. This work reports the energy storage material cost (\$/kWh) of various PCMs with phase change between 0 – 65°C. Four PCM classes are analyzed for their potential use in building systems: 1) inorganic salt hydrates, 2) organic fatty acids, 3) organic fatty alcohols, and 4) organic paraffin waxes. Many salt hydrates have low material costs (0.09 – 2.53 \$/kg), high latent heat of fusion (100 – 290 J/g), and high densities (1.3 – 2.6 g/cm<sup>3</sup>), leading to favorable volumetric storage density and low energy storage costs, 50 – 130 kWh/m<sup>3</sup> and 0.90 – 40 \$/kWh, respectively. Some salts are notably more expensive due to their scarcity or pressures from competing industries such as lithium-based salts. Fatty acids have the lowest energy storage cost in the temperature range 8 – 17°C at 6.50 – 40 \$/kWh. Despite favorable latent heat (125 – 250 J/g) their low density gives (0.9 g/cm<sup>3</sup>) gives poor volumetric storage capacity, 32 – 80 kWh/m<sup>3</sup>. Fatty alcohols generally have high material costs 2.50 – 200 \$/kg which leads to high energy storage costs, 40 – 3000 \$/kWh. With latent heat and density similar to fatty acids, fatty alcohols have poor volumetric energy storage, 43 – 55 kWh/m<sup>3</sup>. Paraffin waxes containing only a single length carbon chain have a higher energy cost (15 – 500 \$/kWh) than generic paraffin waxes containing many lengths of carbon chains (7 – 30 \$/kWh). Pure waxes have a discrete phase change temperature due to their homogeneity. In contrast, a less refined generic wax with several carbon chain lengths is more likely to have a pronounced temperature glide during its phase change. Pure single carbon chain waxes are generally required for applications <45°C as generic paraffin waxes melt between 45 – 70°C. For many waxes, a solid-solid transition occurs at temperatures below the solid-liquid phase change. For pure paraffins with carbon content  $\geq 22$  C atoms, these transitions may appear near the same temperature resembling a temperature glide. The challenges with fatty acids, fatty alcohols, and waxes are low thermal conductivity, low density, some flammability concerns, and compatibility issues with some common engineering materials such as polymers. Challenges with salt hydrates are pronounced supercooling (>5°C), incongruent melting, and corrosiveness. All PCMs may degrade if exposed to ambient conditions and therefore require proper sealing.

### 1. INTRODUCTION

A phase change material (PCM) is capable of absorbing, storing, and releasing thermal energy nearly isothermally at the phase change temperature. The thermal battery may act as a heat source or a heat sink depending on the desired application, mode of operation, and the phase change temperature. The selection of a PCM for a given application is dependent on its phase change temperature, the size of the system, the external operating temperatures, and cost.

Incorporating PCMs into building systems has been researched extensively. There are two schemes of incorporating PCMs into building systems: 1) passive systems whereby the PCM acts as an unobtrusive and uncontrolled thermal

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buffer for high transient thermal loads on the building envelope, and 2) active systems where the PCM is coupled to a heat pump or similar mechanical device and absorbs or releases heat at the operators' control. The successful implementation of both passive and active systems requires a PCM with an appropriate phase change temperature.

The present study examines the thermophysical properties of PCMs with a phase change temperature of 0 – 65°C that may be useful for building applications: inorganic salt hydrates, organic fatty acids, organic fatty alcohols, and organic paraffin waxes. This present study expands on the work published by Hirshey et al. (2018).

## 2. PCM PROPERTIES

### 2.1 Inorganic Salt Hydrate PCMs

Salt hydrates are inorganic materials composed of salt and water in specific molar ratios. The salt and water form a solid crystalline structure, often different than the original salt crystal structure. Some salts may form multiple hydrates with different water:salt ratios. The solid-liquid phase change process for a salt hydrate is observed when the hydrogen bonds between the water molecules in the solid crystal structure are overcome by the molecular vibrations and the water is liberated from the crystal structure forming an aqueous solution. In many salt hydrates the salt is not fully soluble in the water content of its hydrate. This results in incongruent melting whereby the undissolved salt settles out of the solution.

The liquid-solid phase change for a salt hydrate is the reformation of the salt hydrate crystal structure from the aqueous solution. However, many salt hydrates experience extreme supercooling which is the phenomenon where the liquid cool below nominal phase change temperature without the spontaneous formation of the solid structure. Supercooling can be problematic for systems that rely on a consistent phase change temperature. Solutions to preventing large supercooling include adding nucleating agents or through some mechanical work (shaking, vibrating, stirring) (Lane, 1992). Some systems may take advantage of this supercooling phenomenon into the design; the subcooled liquid salt hydrate is stored nearer the ambient temperature, removing the need for insulation and recrystallization provided from an exterior source when the heat release is desired (Sandnes & Rekstad, 2006).

Incongruently melted salt hydrates are not homogenous; there is a gradient from saturated solution to anhydrous salt. This separation between the water and salt does not allow for the full recrystallization of the original salt hydrate crystal and the resulting smaller crystal will form a barrier between water and anhydrous salt. This leads to a reduction in energy storage capacity as only a fraction of the original PCM will crystallize. In a closed system, the full solid salt hydrate may recrystallize, but the time required is not useful for thermal storage systems.

Salt hydrates have been explored extensively for their thermal storage potential, namely high volumetric latent heat. Table 1 shows the thermal energy storage-relevant thermophysical properties of salt hydrates including nominal phase change temperature (solid-to-liquid phase change; the degree of supercooling can be unpredictable), the latent heat associated with the phase change, and the solid density. Some double salts are included in this analysis. Double salts are those salts with two cation or two anions in the unit cell, but the resultant is distinct in the crystal structure and properties than the corresponding salts with only single cations or anions, e.g., chromium (III) potassium sulfate dodecahydrate ( $\text{CrK}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ ).

### 2.2 Organic PCMs

Organic PCMs are materials that consist of a hydrocarbon chain. Organic PCMs include, but are not limited to, waxes, alcohols, and fatty acids. The phase transition temperature of organic PCMs often correlates to its hydrocarbon chain length. For most saturated organic compounds, a longer chain has higher melting temperatures. Unsaturated or branched organic compounds may break from this simplification. Organic PCMs may exhibit a temperature glide where the phase change occurs over a temperature range around the nominal phase change temperature. Often the reported enthalpy values for these materials with glide include the sensible heating that is present in the glide. Some organic PCMs may display supercooling tendencies where the temperature for the onset of freezing occurs below the temperature for the completion of melting. This is observed more frequently in unsaturated materials or those that contain many polymorphic forms. These are often more predictable and repeatable than supercooling of salt hydrate PCMs. Only the solid-to-liquid phase change temperatures are reported here. Unsaturated hydrocarbons are less stable than similar saturated chains and thus are more susceptible to oxidation. Therefore, proper sealing and separation from atmospheric oxygen is required if these materials are used

for TES without degradation. Most organic PCMs are biodegradable. Some material compliance issues with plastics and polymers may be present for some organic PCMs.

## 2.4 Fatty Acid PCMs

Fatty acids are a subset of carboxylic acids which have an organic functional group terminating with a carboxyl group and have the general formula R-COOH. The functional group for a fatty acid is generally a hydrocarbon chain, saturated or unsaturated. Saturated fatty acids may be written as  $\text{COOH}(\text{CH}_2)_n\text{CH}_3$ . Fatty acids are named so because they are the basis of the fats of all plants and animals; a triglyceride is composed of glycerol and three fatty acids. The most commonly analyzed fatty acids for TES are medium to long straight-chain saturated fatty acids with an even number of carbon atoms: capric acid (C10:0), lauric acid (C12:0), myristic acid (C14:0), palmitic acid (C16:0), and stearic acid (C18:0). Fatty acids with an odd number of carbon atoms exist, albeit more rarely, and will be included in this analysis when data is available. For completeness and comparison, formic acid ( $\text{HCOOH}$ ) and acetic acid ( $\text{CH}_3\text{COOH}$ ) are included in this analysis as they contain the same terminating carboxyl group although they do not appear in naturally occurring triglycerides.

## 2.5 Fatty Alcohol PCMs

The fatty alcohols analyzed here are primary alcohols composed of a saturated or unsaturated hydrocarbon chain terminating with an alcohol group and have the general formula R-OH. Saturated fatty alcohols are written as  $\text{CH}_3(\text{CH}_2)_n\text{OH}$ . More alcohols exist with branches and additional functional groups, but these will be excluded.

## 2.5 Paraffin Waxes

Paraffin waxes are common for thermal energy storage, are often derived from petroleum sources. Paraffins are straight-chain, saturated alkane hydrocarbons with no terminating functional groups, written as  $\text{C}_n\text{H}_{2n+2}$ . More detail on paraffin structure is included in Hirshey et al. (2018). Many paraffins have a solid-solid transition at a lower temperature than the solid-liquid transition. The crystalline solid structures vary by the carbon content, more details included in Mondieig et al. (2004). In paraffins with a carbon number  $\geq 22$ , the solid-solid transition temperature,  $T_{s-s}$ , may be very near the solid-liquid transition,  $T_{s-l}$ . For example, tetracosane ( $\text{C}_{24}\text{H}_{50}$ ) has  $T_{s-s} \approx 48^\circ\text{C}$  and a  $T_{s-l} \approx 50.3^\circ\text{C}$ . The latent heat associated with the solid-solid is nearly 90 J/g and the solid-liquid is around 160 J/g. Thus, tetracosane may be considered as having a total latent heat 250 J/g with a  $2.3^\circ\text{C}$  temperature glide if both transitions are included. This analysis will show solid-solid and solid-liquid separately where data is available.

The predominant application for paraffins with melting temperatures between 50 – 70°C is candle making. These waxes are not pure substances, rather they are a mix of several alkane chains of various lengths with a marketed average melting temperature. Due to their heterogeneity, these waxes may have several degrees of temperature glide. Often the exact chemical composition is unknown. The melting temperature of these candle making waxes generally overlap with pure paraffins with a carbon content between 24 and 32 atoms but at a reduced cost.

## 3. METHODOLOGY

The thermophysical properties of the PCMs are surveyed from literature. When available, a primary source and measurement data were used. Many reported PCM thermophysical properties have “citation chains” where the same values are repeated article after article. Attempts were made to trace back to the original measurement data which are often old, difficult to locate, or used out-of-date technology; or search for more recent data. Where primary data was not found, a (\*) is denoted by the material name. These PCMs should be viewed more critically, and more work should be done to assess their viability and confirm these data. Materials in the tables but not present in Figure 1 have current costs that exceed the maximum value of the chart.

All cost data were gathered from data publicly available from industrial suppliers using the CAS number as the search terms. Wherever possible, the cost data were collected in bulk quantities per metric ton or per ton. Several different suppliers for each PCM were identified and the listed prices recorded. Care was taken to ensure that the same material form was used for each individual material to ensure an accurate cost comparison (e.g. powder). All cost data is consolidated into a single dataset source white paper, Hirshey (2020). All cost data were collected in the autumn of 2020 and prices were largely static during this time. Some seasonality may exist for materials that have seasonal applications such as calcium chloride ( $\text{CaCl}_2$ ) as a deicing agent.

Salt hydrates were sourced in their anhydrous form and the cost of water was considered negligible. Many salt hydrates with other industrial applications may only be sold as a solution with water, e.g. calcium bromide ( $\text{CaBr}_2$ ) as a 52% solution drilling fluid. Under these special circumstances, the PCM cost was adjusted by the stoichiometric anhydrous salt content. It should be noted that adding water in bulk to some anhydrous salts can be an energetic exothermic event, and proper safety precautions should be taken. This reaction is distinct from, though related to, the solid-liquid phase transformations analyzed here.

The energy storage material cost was calculated by dividing the material bulk cost (\$/kg) by melting enthalpy (kJ/kg), and plotted versus the material melting temperature in Figure 1. The vertical error bars represent the range of possible energy storage material costs which includes extrema in price and melting enthalpy values. Many material costs vary wildly, sometimes two orders of magnitude. This is often the difference between ordering a single shipment of one metric ton versus regular shipments of hundreds of metric tons.

The horizontal error bars of Figure 1 represent the range in documented melting temperatures of that material; they do not represent supercooling or temperature glide. For materials that experience a temperature glide, the peak temperature, or similar, is used. The peak temperature is the temperature that shows a maximum value in a heat flow vs. temperature curve (commonly differential scanning calorimetry data). This temperature may vary with the experimental variables.

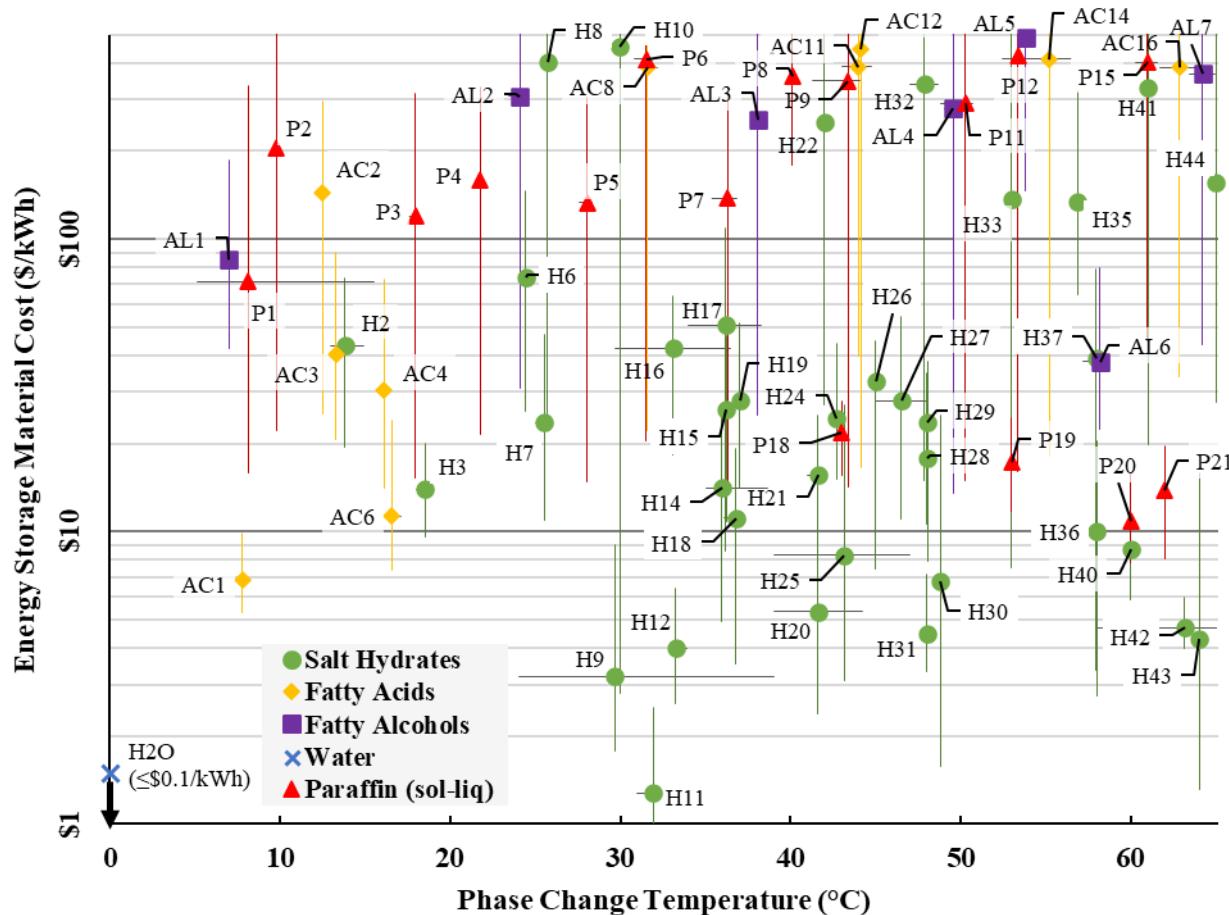


Figure 1: PCM Energy Storage Material Cost

**Table 1:** Properties of Salt Hydrate PCMs

<b>Fig. 1 ID</b>	<b>Salt Hydrate</b>	<b>Chemical Formula</b>	<b>Anhydrous Salt CAS Number</b>	<b>Melting Temp (°C)</b>	<b>Melting Enthalpy (J/g)</b>	<b>Density (kg/m<sup>3</sup>)</b>	<b>Cost (\$/kg)</b>	<b>Thermophysical property sources</b>
-	Lithium Chlorate Trihydrate	LiClO <sub>3</sub> ·3H <sub>2</sub> O	13453-71-9	8.0 – 8.2	155 – 253.0	1720	25.00 - 37.50	(Gawron & Shröder, 1977; Guion et al., 1983; Marcus, 2017)
H2	Dipotassium Hydrogen Phosphate Hexahydrate*	K <sub>2</sub> HPO <sub>4</sub> ·6H <sub>2</sub> O	7758-11-4	13.0 – 15.0	107 – 122.0	2440	0.66 - 1.34	(Guion et al., 1983; Kauffman & Pan, 1973; Marcus, 2017)
H3	Potassium Fluoride Tetrahydrate	KF·4H <sub>2</sub> O	7789-23-3	18.0 – 18.9	231 – 330	1445	0.88 - 1.00	(Couniou & Cohen-Adad, 1976; Guion et al., 1983; S. D. Sharma et al., 2004)
-	Sodium Chromate Decahydrate*	Na <sub>2</sub> CrO <sub>4</sub> ·10H <sub>2</sub> O	7775-11-3	16.0 – 18.9	164 – 172	1483	10.00 - 51.67	(Guion et al., 1983; Kauffman & Pan, 1973)
-	Iron (III) Bromide Hexahydrate*	FeBr <sub>3</sub> ·6H <sub>2</sub> O	10031-26-2	21.0 – 27	105	1820	10.00 - 119.33	(S. D. Sharma et al., 2004; Veerakumar & Sreekumar, 2016)
H6	Copper (II) Nitrate Hexahydrate	Cu(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	3251-23-8	24.4	123	2074	0.88 - 2.53	(Guion et al., 1983; Kauffman & Pan, 1973)
H7	Manganese (II) Nitrate Hexahydrate	Mn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	10377-66-9	25.0 – 26.0	125.8 – 148	1800	0.45 - 0.89	(Marcus, 2017; Nagano et al., 2003)
H8	Lithium Metaborate Octahydrate*	LiBO <sub>2</sub> ·8H <sub>2</sub> O	13453-69-5	25.7	289	1400	2.00 - 32.33	(S. D. Sharma et al., 2004)
H9	Calcium Chloride Hexahydrate	CaCl <sub>2</sub> ·6H <sub>2</sub> O	10043-52-4	24 – 30.0	133.9 – 211.3	1710	0.10 - 0.19	(Guion et al., 1983)
H10	Lithium Nitrate Trihydrate	LiNO <sub>3</sub> ·3H <sub>2</sub> O	7790-69-4	29.9 – 30.0	189 – 296	1575	0.23 - 37.43	(Guion et al., 1983; Kauffman & Pan, 1973; S. D. Sharma et al., 2004)
H11	Sodium Sulfate Decahydrate	Na <sub>2</sub> SO <sub>4</sub> ·10H <sub>2</sub> O	7757-82-6	31.0 – 32.4	239 – 251.2	1477	0.03 - 0.09	(Abhat, 1983; S. D. Sharma et al., 2004)
H12	Sodium Carbonate Decahydrate	Na <sub>2</sub> CO <sub>3</sub> ·10H <sub>2</sub> O	497-19-8	33.0 – 33.9	179.8 – 251	1447	0.18 - 0.26	(Guion et al., 1983; Rao et al., 2018)
-	Lithium Bromide Dihydrate*	LiBr <sub>2</sub> ·2H <sub>2</sub> O	7550-35-8	34	124	1570	1.00 - 20.67	(S. D. Sharma et al., 2004)
H14	Sodium Hydrogen Phosphate Dodecahydrate	Na <sub>2</sub> HPO <sub>4</sub> ·12H <sub>2</sub> O	7558-79-4	35.0 – 38.7	187.7 – 281	1521	0.39 - 1.03	(Abhat, 1983; Guion et al., 1983; Lorsch et al., 1975; Rao et al., 2018)
H15	Zinc Nitrate Hexahydrate	Zn(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	7779-88-6	36.0 – 36.4	126.7 – 147	2015	0.44 - 0.99	(Abhat, 1983; Lorsch et al., 1975; Marcus, 2017; Rao et al., 2018)
H16	Ammonium Iron (III) Sulfate Dodecahydrate*	FeNH <sub>4</sub> (SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	10138-04-2	29.7 – 36.5	197.6	1713	1.00 - 2.32	(Guion et al., 1983)
H17	Calcium Bromide Hexahydrate	CaBr <sub>2</sub> ·6H <sub>2</sub> O	7789-41-5	34.0 – 38.3	115 – 138	2228	0.28 - 1.64	(Marcus, 2017; S. D. Sharma et al., 2004)
H18	Iron (III) Chloride Hexahydrate	FeCl <sub>3</sub> ·6H <sub>2</sub> O	7705-08-0	36.1 – 37.0	186.2 – 226	1600	0.22 - 0.68	(Guion et al., 1983; Kauffman & Pan, 1973; Marcus, 2017)
H19	Manganese (II) Nitrate tetrahydrate*	Mn(NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	10377-66-9	37.0	115	2130	0.45 - 0.89	(S. D. Sharma et al., 2004)
H20	Calcium Chloride Tetrahydrate	CaCl <sub>2</sub> ·4H <sub>2</sub> O	10043-52-4	39 – 44.2	99.6 – 158	1567	0.10 - 0.19	(S. D. Sharma et al., 2004)
H21	Potassium Fluoride Dihydrate*	KF·2H <sub>2</sub> O	7789-23-3	41.0 – 42.0	162 – 266	1658	0.88 - 1.00	(Guion et al., 1983; S. D. Sharma et al., 2004)
H22	Magnesium Iodide Octahydrate*	MgI <sub>2</sub> ·8H <sub>2</sub> O	10377-58-9	42	133	2098	1.00 - 9.30	(S. D. Sharma et al., 2004)
-	Calcium Iodide Hexahydrate*	CaI <sub>2</sub> ·6H <sub>2</sub> O	10102-68-8	42	162	2550	20.00 - 76.75	(S. D. Sharma et al., 2004)
H24	Chromium (III) Potassium Sulfate Dodecahydrate*	CrK(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	10141-00-1	42.7	237.9	1828	1.00 - 1.61	(Guion et al., 1983)
H25	Calcium Nitrate Tetrahydrate	Ca(NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	10124-37-5	39.0 – 47.0	106 – 209.2	1858	0.18 - 0.34	(Guion et al., 1983; Kauffman & Pan, 1973; S. D. Sharma et al., 2004)
H26	Tripotassium Phosphate Heptahydrate*	K <sub>3</sub> PO <sub>4</sub> ·7H <sub>2</sub> O	7778-53-2	45	145	2500	0.30 - 1.32	(S. D. Sharma et al., 2004)

**Table 1** (continued): Properties of Salt Hydrate PCMs

Fig. 1 ID	Salt Hydrate	Chemical Formula	Anhydrous Salt CAS Number	Melting Temp (°C)	Melting Enthalpy (J/g)	Density (kg/m <sup>3</sup> )	Cost (\$/kg)	Thermophysical property sources
H27	Zinc Nitrate Tetrahydrate*	Zn(NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	7779-88-6	45 – 48.0	110 – 144	2220	0.44 - 0.99	(Guion et al., 1983; S. D. Sharma et al., 2004)
H28	Sodium Metasilicate Pentahydrate*	Na <sub>2</sub> SiO <sub>3</sub> ·5H <sub>2</sub> O	6834-92-0	48.0	68	2610	0.20 - 0.34	(S. D. Sharma et al., 2004)
H29	Sodium Hydrogen Phosphate Heptahydrate	Na <sub>2</sub> HPO <sub>4</sub> ·7H <sub>2</sub> O	7558-79-4	48.0 – 48.2	135 – 170	1679	0.39 - 1.03	(Guion et al., 1983; Kauffman & Pan, 1973; S. D. Sharma et al., 2004)
H30	Magnesium Sulfate Heptahydrate*	MgSO <sub>4</sub> ·7H <sub>2</sub> O	7487-88-9	48 – 49.2	201 – 202	1680	0.09 - 0.46	(Guion et al., 1983; Kauffman & Pan, 1973; S. D. Sharma et al., 2004)
H31	Sodium thiosulfate pentahydrate	Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> ·5H <sub>2</sub> O	7772-98-7	48.0	200 – 209	1708	0.19 - 0.25	(Bajnóczy et al., 1995; Zhang et al., 1999)
H32	Iron Nitrate Nonahydrate*	Fe(NO <sub>3</sub> ) <sub>3</sub> ·9H <sub>2</sub> O	10421-48-4	47 – 48.7	155 – 190.5	1684	0.79 - 17.91	(Guion et al., 1983; S. D. Sharma et al., 2004)
H33	Sodium Nitrate Hexahydrate*	NaNO <sub>3</sub> ·6H <sub>2</sub> O	7631-99-4	53.0	158	2261	0.33 - 6.02	(Guion et al., 1983)
-	Cobalt Nitrate Hexahydrate*	Co(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	10141-05-6	55.5 – 57.0	115 – 203.3	1870	1.00 - 23.50	(Marcus, 2017; S. D. Sharma et al., 2004)
H35	Nickel Nitrate Hexahydrate*	Ni(NO <sub>3</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	13138-45-9	56.7 – 57	168	2050	3.00 - 6.25	(Guion et al., 1983; S. D. Sharma et al., 2004)
H36	Sodium Acetate Trihydrate	CH <sub>3</sub> COONa·3H <sub>2</sub> O	127-09-3	57.9 – 58.0	180 – 289	1450	0.22 - 0.71	(Bajnóczy et al., 1995; Marcus, 2017)
H37	Manganese Chloride Tetrahydrate*	MnCl <sub>2</sub> ·4H <sub>2</sub> O	7773-01-5	57.9 – 58.0	151 – 178	2010	0.17 - 1.84	(Guion et al., 1983; S. D. Sharma et al., 2004)
-	Lithium Acetate Dihydrate*	CH <sub>3</sub> COOLi·2H <sub>2</sub> O	546-89-4	57.9 – 58.0	250.9 – 377	1300	3.00 - 59.15	(Marcus, 2017; S. D. Sharma et al., 2004)
-	Cadmium Nitrate Tetrahydrate*	Cd(NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	10325-94-7	59 – 59.5	98 – 155	1773	10.00 - 45.00	(Guion et al., 1983; Marcus, 2017; S. D. Sharma et al., 2004)
H40	Sodium Bisulfate Monohydrate*	NaHSO <sub>4</sub> ·H <sub>2</sub> O	7681-38-1	60	129.6	1800	0.21 - 0.31	(Guion et al., 1983)
H41	Sodium Aluminum Sulfate Dodecahydrate*	NaAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	10102-71-3	61	181	1675	1.00 - 16.63	(S. D. Sharma et al., 2004)
H42	Sodium Hydroxide Monohydrate	NaOH·H <sub>2</sub> O	1310-73-2	58 – 65.2	272 – 272.4	1710	0.30 - 0.36	(Murch & Giauque, 1962; S. D. Sharma et al., 2004)
H43	Iron (II) Sulfate Heptahydrate*	FeSO <sub>4</sub> ·7H <sub>2</sub> O	7720-78-7	64.0	200	1890	0.07 - 0.24	(Guion et al., 1983)
H44	Chromium Nitrate Nonahydrate*	Cr(NO <sub>3</sub> ) <sub>3</sub> ·9H <sub>2</sub> O	13548-38-4	65.0	194.8	1807	1.50 - 8.46	(Guion et al., 1983)

\* Single primary measurement or no primary measurement found

**Table 2:** Properties of Fatty Alcohols PCMs

Fig. 1 ID	Fatty Alcohol	Chemical Formula	CAS Number	Melting Temperature (°C)	Melting Enthalpy (J/g)	Density (kg/m <sup>3</sup> )	Cost (\$/kg)	Thermophysical property sources
AL1	1-Decanol	C <sub>10</sub> H <sub>22</sub> O	112-30-1	6.7 – 7.5	181 – 212	830	2.5 – 9.36	(de Matos et al., 2015)
AL2	Lauryl alcohol	C <sub>12</sub> H <sub>26</sub> O	112-53-8	23.2 – 24.7	202 – 216	831	1.85 – 100	(de Matos et al., 2015; Saeed et al., 2016; van Miltenburg et al., 2003)
AL3	Myristyl alcohol	C <sub>14</sub> H <sub>30</sub> O	112-72-1	37.9 – 38.2	219 – 230	824	1.60 – 80	(Maximo et al., 2014)
AL4	Cetyl alcohol	C <sub>16</sub> H <sub>34</sub> O	36653-82-4	49 – 50.1	232 – 240	811	0.90 – 50	(Maximo et al., 2014)
AL5	Heptadecyl alcohol	C <sub>17</sub> H <sub>36</sub> O	1454-85-9	53.4 – 54.1	244 – 245.8	815	10 – 100	(van Miltenburg et al., 2003; Ventolà et al., 2004)
AL6	Stearyl alcohol	C <sub>18</sub> H <sub>38</sub> O	112-92-5	57.2 – 58.7	148 – 257	813	1.60 – 3.30	(Maximo et al., 2014; van Miltenburg et al., 2001; Ventolà et al., 2004)
AL7	Arachidyl alcohol	C <sub>20</sub> H <sub>42</sub> O	629-96-9	63.5 – 65	241 – 247	805	3 – 199	(van Miltenburg et al., 2001; Ventolà et al., 2004)

**Table 3:** Properties of Fatty Acid PCMs

Fig. 1 ID	Fatty Acid	Structural Chemical Formula	CAS Number	Melting Temperature (°C)	Melting Enthalpy (J/g)	Density (kg/m³)	Cost (\$/kg)	Thermophysical property sources
AC1	Formic Acid Methanoic Acid	HCOOH	64-18-6	7.8 – 8.4	247	1200	0.36 - 0.68	(Veerakumar & Sreekumar, 2016)
AC2	Pelargonic Acid Nonanoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> COOH	112-05-0	12.5	128	900	0.90 - 10.60	(Acree, 1991)
AC3	α-Oleic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH=CH(CH <sub>2</sub> ) <sub>7</sub> COOH	112-80-1	13.3	76 – 140	895	0.80 - 3.50	(Acree, 1991; Cedeño et al., 2001; Sato et al., 1997)
AC4	β-Oleic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH=CH(CH <sub>2</sub> ) <sub>9</sub> COOH	112-80-1	16.0 – 16.3	173 – 205	895	0.80 - 3.50	(Cedeño et al., 2001; Sato et al., 1997)
-	Caprylic Acid Octanoic acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> COOH	124-07-2	16.3 – 16.7	135 – 148	910	3.50 - 120.00	(Acree, 1991; Domalski & Hearing, 1996)
AC6	Acetic Acid Ethanoic Acid	CH <sub>3</sub> COOH	64-19-7	16 – 16.91	180 – 195	1270	0.40 - 1.20	(Julius, 1910; Parks & Kelley, 1925; Pickering, 1895)
-	Undecylic Acid Undecanoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>9</sub> COOH	112-37-8	28.6	139	890	1 - 5	(Domalski & Hearing, 1996)
AC8	Capric Acid Decanoic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> COOH	334-48-5	31 – 32.13	152.7 – 162.7	885	1 - 100	(Hobi Bordón Sosa et al., 2019; Saeed et al., 2016; A. Sharma et al., 2005)
-	Petroselinic Acid o-6-0ctadecenoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> CH=CH(CH <sub>2</sub> ) <sub>4</sub> COOH	593-39-5	30.5	168	900	10 - 100	(Sato et al., 1997)
-	Tridecylic Acid Tridecanoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>11</sub> COOH	638-53-9	41.5	157	983	20 - 150	(Domalski & Hearing, 1996)
AC11	Lauric Acid Dodecanoic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> COOH	143-07-7	44 – 44.92	177.4 – 181.5	903	2.00 - 200	(Hobi Bordón Sosa et al., 2019; Saeed et al., 2016; A. Sharma et al., 2005)
AC12	Elaidic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH=CH(CH <sub>2</sub> ) <sub>7</sub> COOH	112-79-8	43.9 – 44.5	190 – 218	873	1 - 50	(Wilson et al., 2015)
-	Pentadecanoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>13</sub> COOH	1002-84-2	52.5	188	842	50 - 150	(Wilson et al., 2015)
AC14	Myristic Acid Tetradecanoic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>12</sub> COOH	544-63-8	54.2 – 58	191 – 198	962	1 - 120	(Hobi Bordón Sosa et al., 2019; Saeed et al., 2016; A. Sharma et al., 2005)
-	Margaric Acid Heptadecanoic Acid*	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> COOH	506-12-7	61.2 – 61.3	217	853	2500 - 7500	(Wilson et al., 2015)
AC16	Palmitic Acid Hexadecanoic Acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOH	57-10-3	62.5 – 64	163 – 212	886	2 - 150	(Hobi Bordón Sosa et al., 2019; Saeed et al., 2016; A. Sharma et al., 2005)

\* Single primary measurement or no primary measurement found

**Table 4:** Properties of Paraffin PCMs

Fig 1 ID	Paraffin Name	Chemical Formula	CAS Number	Dominant Solid-Solid Temp (°C)	Solid-Solid Enthalpy (J/g)	Solid-Liquid Temp (°C)	Solid-Liquid Enthalpy (J/g)	Density (kg/m³)	Cost (\$/kg)	Thermophysical property sources
P1	Tetradecane	C <sub>14</sub> H <sub>30</sub>	629-59-4	-79	0.9	5.2 - 15.6	215 - 227	759	1 - 20	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P2	Pentadecane	C <sub>15</sub> H <sub>32</sub>	629-62-9	-3 - -2	41 - 43	9.6 - 10.0	161 - 163	765	1 - 45	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P3	Hexadecane	C <sub>16</sub> H <sub>34</sub>	544-76-3	-	-	17.6 - 18.2	228 - 236	770	1 - 20	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P4	Heptadecane	C <sub>17</sub> H <sub>36</sub>	629-78-7	11	45 - 46	21.6 - 22.0	164 - 167	775	1 - 15	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P5	Octadecane	C <sub>18</sub> H <sub>38</sub>	593-45-3	-	-	27.6 - 28.4	236 - 242	779	1 - 20	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P6	Nonadecane	C <sub>19</sub> H <sub>40</sub>	629-92-5	22 - 23	47 - 51	30.8 - 32.0	159 - 176	782	1 - 100	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P7	Icosane	C <sub>20</sub> H <sub>42</sub>	112-95-8	-	-	35.4 - 36.9	218 - 251	785	1 - 20	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P8	Heneicosane	C <sub>21</sub> H <sub>44</sub>	629-94-7	31 - 33	52 - 56	39.9 - 40.3	155 - 161	788	8 - 100	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P9	Docosane	C <sub>22</sub> H <sub>46</sub>	629-97-0	40 - 43	29 - 128	41.3 - 44.1	49 - 253	791	1 - 25	(Domalski & Hearing, 1996; Mondieig et al., 2004)
-	Tricosane	C <sub>23</sub> H <sub>48</sub>	638-67-5	39 - 41	60 - 67	46.6 - 47.7	161 - 236	793	1 - 100	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P11	Tetracosane	C <sub>24</sub> H <sub>50</sub>	646-31-1	46 - 51	82 - 93	48.9 - 50.7	159 - 241	796	1 - 25	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P12	Pentacosane	C <sub>25</sub> H <sub>52</sub>	629-99-2	47 - 53	67 - 75	53.1 - 53.6	160 - 225	798	1 - 100	(Domalski & Hearing, 1996; Mondieig et al., 2004)
-	Hexacosane	C <sub>26</sub> H <sub>54</sub>	630-01-3	50 - 53	83 - 95	56.0 - 56.5	160 - 174	800	15,620	(Domalski & Hearing, 1996; Mondieig et al., 2004)
-	Heptacosane	C <sub>27</sub> H <sub>56</sub>	593-49-7	47 - 53	71 - 76	58.5 - 58.8	159 - 165	802	255,000	(Domalski & Hearing, 1996; Mondieig et al., 2004)
P15	Octacosane	C <sub>28</sub> H <sub>58</sub>	630-02-4	56 - 58	85 - 90	60.3 - 61.6	160 - 169	803	2.10 - 100	(Domalski & Hearing, 1996; Mondieig et al., 2004)
-	Nonacosane	C <sub>29</sub> H <sub>60</sub>	630-03-5	58 - 58	73 - 73	63.4	162	805	10 - 100	(Domalski & Hearing, 1996)
-	Triacontane	C <sub>30</sub> H <sub>62</sub>	638-68-6	59 - 62	86 - 89	65.5 - 65.6	163	806	16,800	(Domalski & Hearing, 1996)
P18	Paraffin 46-50	-	-	20	-	43.0	228	765	0.99 - 1.76	(Ukrainczyk et al., 2010)
P19	Paraffin 52-54	-	-	20	-	53.0	220	774	0.72 - 1.50	(Ukrainczyk et al., 2010)
P20	Paraffin 58-62	-	-	27	-	60.0	206	782	0.45 - 0.90	(Ukrainczyk et al., 2010)
P21	Paraffin 62-70	-	-	25	-	62.0	201	799	0.45 - 1.10	(Ukrainczyk et al., 2010)

## 4. CONCLUSIONS

- Salt hydrate PCMs have the lowest energy storage cost for applications 18 – 65°C, between 0.90 – 15 \$/kWh. With high density and latent heat, salt hydrates have the highest volumetric energy storage, 50 – 130 kWh/m<sup>3</sup>.
- Fatty acid PCMs have the lowest energy storage cost in 8 – 17°C range, between 6.50 – 40 \$/kWh. Fatty acids with higher melting temperatures are scarcer and thus have higher costs comparable to other organics.
- Organic fatty alcohols have the highest average energy storage cost, >40 \$/kWh, for all temperatures.
- Pure paraffin waxes consisting of a single length carbon chain may be viable for applications between 8 – 28°C with energy storage costs 16 – 25 \$/kWh at their most competitive material costs.
- Generic paraffin waxes that have many different carbon chains of various lengths are more viable for applications 40 – 65°C, at 7 – 30 \$/kWh, but these materials have more pronounced temperature glide.

## REFERENCES

Abhat, A. (1983). Low temperature latent heat thermal energy storage: Heat storage materials. *Solar Energy*, 30(4), 313-332.

Acree, W. E. (1991). Thermodynamic properties of organic compounds: enthalpy of fusion and melting point temperature compilation. *Thermochimica Acta*, 189(1), 37-56.

Bajnóczy, G., Gagyi Pálffy, E., Prépostffy, E., & Zöld, A. (1995). Thermal Properties of a Heat Storage Device Containing Sodium Acetate Trihydrate. *Periodica Polytechnica Chemical Engineering*, 39(2), 129-135.

Cedeño, F. O., Prieto, M. a. M., Espina, A., & García, J. R. (2001). Measurements of temperature and melting heat of some pure fatty acids and their binary and ternary mixtures by differential scanning calorimetry. *Thermochimica Acta*, 369(1), 39-50.

Counioux, J.-J., & Cohen-Adad, R. (1976). Détermination, par calorimétrie du chute, des enthalpies de fusion des hydrates à fusion congruente du ternaire KOH-KF-H<sub>2</sub>O. *Bulletin de la Société chimique de France*, 373-376.

de Matos, F. C., da Costa, M. C., de Almeida Meirelles, A. J., & Batista, E. A. C. (2015). Binary solid-liquid equilibrium systems containing fatty acids, fatty alcohols and triolein by differential scanning calorimetry. *Fluid Phase Equilibria*, 404, 1-8.

Domalski, E. S., & Hearing, E. D. (1996). Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume III. *Journal of Physical and Chemical Reference Data*, 25(1), 1-525.

Gawron, K., & Shröder, J. (1977). Properties of some salt hydrates for latent heat storage. *International Journal of Energy Research*, 1(4), 351-363.

Guion, J., Sauzade, J. D., & Laugt, M. (1983). Critical Examination and Experimental Determination of Melting Enthalpies and Entropies of Salt Hydrates. *Thermochimica Acta*, 67, 167-179.

Hirschey, J. (2020). *PCM Cost*. Retrieved from: [https://web.archive.org/web/20201216164857/https://drive.google.com/file/d/1-LceoENyhh5W2jHt9X7f72hQ\\_VyXsnzM/view](https://web.archive.org/web/20201216164857/https://drive.google.com/file/d/1-LceoENyhh5W2jHt9X7f72hQ_VyXsnzM/view)

Hirschey, J., Gluesenkamp, K. R., Mallow, A., & Graham, S. (2018). Review of Inorganic Salt Hydrates with Phase Change Temperature in Range of 5 to 60°C and Material Cost Comparison with Common Waxes.

Hobi Bordón Sosa, F., Dorighello Carareto, N. D., Maximo, G. J., Meirelles, A. J. d. A., & Costa, M. C. (2019). Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry. *Journal of Chemical & Engineering Data*, 64(12), 5017-5027.

Julius, M. (1910). Zur Theorie der Rohrzuckerinversion II. *Zeitschrift für Physikalische Chemie*, 72U(1), 117-123.

Kauffman, K., & Pan, Y.-C. (1973). *Congruently Melting Materials for Thermal Energy Storage in Air Conditioning* (NSF/RANN/SE/GI27976/TR73/5). Retrieved from Philadelphia, PA:

Lane, G. A. (1992). Phase change materials for energy storage nucleation to prevent supercooling. *Solar Energy Materials and Solar Cells*, 27(2), 135-160.

Lorsch, H. G., Kauffman, K. W., & Denton, J. C. (1975). Thermal Energy Storage for Solar Heating and Off-peak Air Conditioning. *Energy Conversion*, 15, 1-8.

Marcus, Y. (2017). Unconventional Deep Eutectic Solvents: Aqueous Salt Hydrates. *ACS Sustainable Chemistry & Engineering*, 5(12), 11780-11787.

Maximo, G. J., Carareto, N. D. D., Costa, M. C., dos Santos, A. O., Cardoso, L. P., Krähenbühl, M. A., & Meirelles, A. J. A. (2014). On the solid-liquid equilibrium of binary mixtures of fatty alcohols and fatty acids. *Fluid Phase Equilibria*, 366, 88-98.

Mondieig, D., Rajabalee, F., Metivaud, V., Oonk, H. A. J., & Cuevas-Diarte, M. A. (2004). n-Alkane Binary Molecular Alloys. *Chemistry of Materials*, 16(5), 786-798.

Murch, L. E., & Giauque, W. F. (1962). THE THERMODYNAMIC PROPERTIES OF SODIUM HYDROXIDE AND ITS MONOHYDRATE. HEAT CAPACITIES TO LOW TEMPERATURES. HEATS OF SOLUTION1. *The Journal of Physical Chemistry*, 66(10), 2052-2059.

Nagano, K., Mochida, T., Kindaichi, S., Domański, R., & Rebow, M. (2003). Thermal characteristics of manganese (II) nitrate hexahydrate as a phase change material for cooling systems. *Applied Thermal Engineering*, 23(2), 229-241.

Parks, G. S., & Kelley, K. K. (1925). THERMAL DATA ON ORGANIC COMPOUNDS. II. THE HEAT CAPACITIES OF FIVE ORGANIC COMPOUNDS. THE ENTROPIES AND FREE ENERGIES OF SOME HOMOLOGOUS SERIES OF ALIPHATIC COMPOUNDS. *Journal of the American Chemical Society*, 47(8), 2089-2097.

Pickering, S. U. (1895). LXXII.—A comparison of some properties of acetic acid and its chloro- and bromo-derivatives. *Journal of the Chemical Society, Transactions*, 67(0), 664-684.

Rao, Z., Xu, T., Liu, C., Zheng, Z., Liang, L., & Hong, K. (2018). Experimental study on thermal properties and thermal performance of eutectic hydrated salts/expanded perlite form-stable phase change materials for passive solar energy utilization. *Solar Energy Materials and Solar Cells*, 188, 6-17.

Saeed, R., Schlegel, J., Castano Giraldo, C., & Sawafta, R. (2016). Uncertainty of Thermal Characterization of Phase Change Material by Differential Scanning Calorimetry Analysis. *International Journal of Engineering Research & Technology*, 5, 405-412.

Sandnes, B., & Rekstad, J. (2006). Supercooling salt hydrates: Stored enthalpy as a function of temperature. *Solar Energy*, 80(5), 616-625.

Sato, K., Yano, J., Kawada, I., Kawano, M., Kaneko, F., & Suzuki, M. (1997). Polymorphic behavior of gondoic acid and phase behavior of its binary mixtures with asclepic acid and oleic acid. *Journal of the American Oil Chemists' Society*, 74(9), 1153-1159.

Sharma, A., Won, L. D., Buddhi, D., & Park, J. U. (2005). Numerical heat transfer studies of the fatty acids for different heat exchanger materials on the performance of a latent heat storage system. *Renewable Energy*, 30(14), 2179-2187.

Sharma, S. D., Kitano, H., & Sagara, K. (2004). *Phase Change Materials for Low Temperature Solar Thermal Applications*.

Ukrainczyk, N., Kurajica, S., & Šipušiæ, J. (2010). Thermophysical Comparison of Five Commercial Paraffin Waxes as Latent Heat Storage Materials. *Chemical and Biochemical Engineering Quarterly*, 24(2), 129-137.

van Miltenburg, J. C., Oonk, H. A. J., & Ventola, L. (2001). Heat Capacities and Derived Thermodynamic Functions of 1-Octadecanol, 1-Nonadecanol, 1-Eicosanol, and 1-Docosanol between 10 K and 370 K. *Journal of Chemical & Engineering Data*, 46(1), 90-97.

van Miltenburg, J. C., van den Berg, G. J. K., & Ramirez, M. (2003). Heat Capacities and Derived Thermodynamic Functions of 1-Dodecanol and 1-Tridecanol between 10 K and 370 K and Heat Capacities of 1-Pentadecanol and 1-Heptadecanol between 300 K and 380 K and Correlations for the Heat Capacity and the Entropy of Liquid n-Alcohols. *Journal of Chemical & Engineering Data*, 48(1), 36-43.

Veerakumar, C., & Sreekumar, A. (2016). Phase change material based cold thermal energy storage: Materials, techniques and applications – A review. *International Journal of Refrigeration*, 67, 271-289.

Ventolà, L., Calvet, T., Cuevas-Diarte, M. A., Ramírez, M., Oonk, H. A. J., Mondieig, D., & Negrier, P. (2004). Melting behaviour in the n-alkanol family. Enthalpy–entropy compensation. *Physical Chemistry Chemical Physics*, 6(8), 1786-1791.

Wilson, J., Gobble, C., & Chickos, J. (2015). Vaporization, Sublimation, and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography. *Journal of Chemical & Engineering Data*, 60(1), 202-212.

Zhang, Y., Jiang, Y., & Jiang, Y. (1999). A simple method, the T-history method, of determining the heat of fusion, specific heat and thermal conductivity of phase-change materials. *Measurement Science and Technology*, 10(3), 201.

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