Supplementary Information

Organic Phase Change Materials for Thermal Energy Storage: Influence of Molecular Structure on Properties

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Table S1. Melting temperatures (T_{fus}) of alkanes with carbon number between 10 and 55. These data were used in Figs. 1 and 2 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	References
$C_{10}H_{22}$	142.28	10	243.50	-29.65	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{11}H_{24}$	156.31	11	247.20	-25.95	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{11}H_{24}$	156.30	11	247.70	-25.45	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{12}H_{26}$	170.33	12	263.50	-9.65	D. D. Tunnicliff and H. Stone, Anal. Chem. 27, 73 (1955). https://doi.org/10.1021/ac60097a022
$C_{12}H_{26}$	170.34	12	263.60	-9.55	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{13}H_{28}$	184.36	13	267.70	-5.45	E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{13}H_{28}$	184.36	13	267.60	-5.55	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{14}H_{30}$	198.39	14	278.30	5.15	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{14}H_{30}$	198.39	14	279.00	5.85	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{15}H_{32}$	212.41	15	282.70	9.55	C. Velez, M. Khayet, and J. M. Ortiz de Zarate, Appl. Energy 143, 383 (2015). https://doi.org/10.1016/j.apenergy.2015.01.054
$C_{15}H_{32}$	212.40	15	283.10	9.95	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{16}H_{34}$	226.44	16	290.90	17.75	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{16}H_{34}$	226.44	16	291.20	18.05	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{17}H_{36}$	240.47	17	294.70	21.55	P. Espeau and J. W. White, Carbon 43, 1885 (2005). https://doi.org/10.1016/j.carbon.2005.02.037
$C_{17}H_{36}$	240.47	17	294.90	21.75	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{18}H_{38}$	254.49	18	300.95	27.80	P. Claudy and J. M. Letoffe, Calorim. Anal. Therm. 22, 281 (1991)
$C_{18}H_{38}$	254.50	18	300.20	27.05	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{19}H_{40}$	268.52	19	305.10	31.95	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{19}H_{40}$	268.52	19	305.00	31.85	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.
$C_{20}H_{42}$	282.55	20	309.70	36.55	V. Metivaud, F. Rajabalee, H. A. J. Oonk, D. Mondieig, and Y. Haget, Can. J. Chem. 77, 332 (1999). https://doi.org/10.1139/v99-004
$C_{20}H_{45}$	282.55	20	310.70	37.55	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	References
$C_{21}H_{44}$	296.57	21	313.00	39.85	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{21}H_{49}$	296.58	21	312.00	38.85	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{22}H_{46}$	310.60	22	316.10	42.95	M. J. S. Monte, A. R. R. P. Almeida, and M. A. V. Ribeiro da Silva, J. Chem. Thermodyn. 36, 385 (2004). https://doi.org/10.1016/j.jct.2004.02.001
$C_{22}H_{46}$	310.60	22	316.95	43.80	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.
$C_{23}H_{48}$	324.63	23	320.20	47.05	L. Robles, D. Mondieig, Y. Haget, and M. A. Cuevas-Diarte, J. Chim. Phys. Phys.-Chim. Biol. 95, 92–111 (1998). https://doi.org/10.1051/jcp:1998111
$C_{23}H_{48}$	324.63	23	319.90	46.75	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{24}H_{50}$	338.65	24	323.80	50.65	E. P. Gilbert, Phys. Chem. Chem. Phys. 1, 1517 (1999). https://doi.org/10.1039/a808664h
$C_{24}H_{50}$	338.66	24	323.00	49.85	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{25}H_{52}$	352.68	25	326.70	53.55	E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{25}H_{52}$	352.69	25	327.40	54.25	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{26}H_{54}$	366.71	26	329.60	56.45	U. Domanska and D. Wyrzykowska-Starkiewicz, Thermochim. Acta 179, 265 (1991). https://doi.org/10.1016/0040-6031(91)80356-N
$C_{26}H_{52}$	366.71	26	328.90	55.75	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{27}H_{56}$	380.73	27	332.00	58.85	E. P. Gilbert, Phys. Chem. Chem. Phys. 1, 1517 (1999). https://doi.org/10.1039/a808664h
$C_{27}H_{56}$	380.74	27	331.20	58.05	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{28}H_{58}$	394.76	28	334.50	61.35	I. Paunovic and A. K. Mehrotra, Thermochim. Acta 356, 27 (2000). https://doi.org/10.1016/S0040-6031(00)00503-7
$C_{28}H_{59}$	394.77	28	333.20	60.05	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{29}H_{60}$	408.79	29	336.80	63.65	E. P. Gilbert, Phys. Chem. Chem. Phys. 1, 1517 (1999). https://doi.org/10.1039/a808664h
$C_{29}H_{60}$	409.79	29	336.00	62.85	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{30}H_{62}$	422.81	30	338.70	65.55	N. V. Platonova, E. N. Kotel'nikova, S. K. Filatov, G. A. Puchkovskaya, I. I. Gnatyuk, J. Baran, and M. Drozd, J. Struct. Chem. 53, 973 (2012). https://doi.org/10.1134/S0022476612050228
$C_{30}H_{62}$	422.82	30	337.50	64.35	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	References
$C_{31}H_{64}$	436.84	31	341.10	67.95	I. Boudouh, I. Djemai, J. A. Gonzalez, and D. Barkat, J. Mol. Liq. 216, 764 (2016). https://doi.org/10.1016/j.molliq.2016.02.010
$C_{31}H_{64}$	436.85	31	340.00	66.85	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{32}H_{66}$	450.87	32	343.50	70.35	E. P. Gilbert, Phys. Chem. Chem. Phys. 1, 1517 (1999). https://doi.org/10.1039/a808664h
$C_{32}H_{66}$	450.87	32	341.90	68.75	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{33}H_{68}$	464.89	33	344.80	71.65	E. P. Gilbert, Phys. Chem. Chem. Phys. 1, 1517 (1999). https://doi.org/10.1039/a808664h
$C_{33}H_{68}$	464.90	33	343.40	70.25	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{34}H_{70}$	478.92	34	346.00	72.85	L. Ventola, M. A. Cuevas-Diarte, T. Calvet, I. Angulo, M. Vivanco, M. Bernar, G. Bernar, M. Melero, and D. Mondieig, J. Phys. Chem. Solids 66, 1668 (2005). https://doi.org/10.1016/j.jpcs.2005.06.001
$C_{34}H_{70}$	478.93	34	345.30	72.15	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{35}H_{72}$	492.95	35	347.20	74.05	H. Yamamoto, S. Teshima, N. Nemoto, and K. Tashiro, J. Phys. Chem. A 113, 2632 (2009). https://doi.org/10.1021/jp808176n
$C_{35}H_{72}$	492.95	35	346.50	73.35	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{36}H_{74}$	506.97	36	348.90	75.75	L. Ventola, M. A. Cuevas-Diarte, T. Calvet, I. Angulo, M. Vivanco, M. Bernar, G. Bernar, M. Melero, and D. Mondieig, J. Phys. Chem. Solids 66, 1668 (2005). https://doi.org/10.1016/j.jpcs.2005.06.001
$C_{36}H_{74}$	506.98	36	348.90	75.75	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{40}H_{82}$	563.08	40	353.20	80.05	L. Ventola, M. A. Cuevas-Diarte, T. Calvet, I. Angulo, M. Vivanco, M. Bernar, G. Bernar, M. Melero, and D. Mondieig, J. Phys. Chem. Solids 66, 1668 (2005). https://doi.org/10.1016/j.jpcs.2005.06.001
$C_{40}H_{82}$	563.08	40	354.00	80.85	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{41}H_{84}$	577.11	41	354.30	81.15	A.-J. Briard, M. Bouroukba, D. Petitjean, N. Hubert, and M. Dirand, J. Chem. Eng. Data 48, 497 (2003). https://doi.org/10.1021/je0201368
$C_{42}H_{86}$	591.13	42	357.30	84.15	M.-H. Wang, Z.-C. Tan, Q. Shi, L.-X. Sun, and T. Zhang, J. Therm. Anal. Calorim. 84, 413 (2006). https://doi.org/10.1007/s10973-005-6971-6
$C_{44}H_{90}$	619.19	44	358.50	85.35	L. Ventola, M. A. Cuevas-Diarte, T. Calvet, I. Angulo, M. Vivanco, M. Bernar, G. Bernar, M. Melero, and D. Mondieig, J. Phys. Chem. Solids 66, 1668 (2005). https://doi.org/10.1016/j.jpcs.2005.06.001
$C_{44}H_{90}$	619.19	44	358.75	85.60	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{46}H_{94}$	647.24	46	360.70	87.55	A.-J. Briard, M. Bouroukba, D. Petitjean, N. Hubert, and M. Dirand, J. Chem. Eng. Data 48, 497 (2003). https://doi.org/10.1021/je0201368
$C_{46}H_{94}$	647.24	46	360.70	87.55	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{50}H_{102}$	703.34	50	365.60	92.45	M. J. Hampden Smith and T. T. Kodas, Chem. Vap. Deposition 1, 8 (1995). https://doi.org/10.1002/cvde.19950010103
$C_{50}H_{102}$	703.34	50	365.25	92.10	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	References
$C_{52}H_{106}$	731.40	52	366.70	93.55	K. Takamizawa, Y. Urabe, J. Fujimoto, H. Ogata, and Y. Ogawa, Thermochim. Acta 267, 297 (1995). https://doi.org/10.1016/0040-6031(95)02487-5
$C_{54}H_{110}$	759.45	54	368.00	94.85	A.-J. Briard, M. Bouroukba, D. Petitjean, N. Hubert, and M. Dirand, J. Chem. Eng. Data 48, 497 (2003). https://doi.org/10.1021/je0201368

Table S2. Thermal properties of alkanes with odd number of carbons. The solid-solid transition temperatures (T_{ss}) and temperatures of fusion (T_{fus}) are listed along with the enthalpies of fusion ($\Delta_{fus}H$) and the total enthalpies of transition ($\Delta_{tot}H = \Delta_{fus}H + \Delta_{ss}H$). These data were used in Figs. 2 and 5 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{ss} (K)	T_{ss} (°C)	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	$\Delta_{tot}H$ (J g^{-1})	References
$C_{11}H_{24}$	156.30	11	-	-	247.70	-25.45	142.20	186.10	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{13}H_{28}$	184.36	13	255.00	-18.15	267.60	-5.55	154.50	196.00	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{15}H_{32}$	212.40	15	270.90	-2.25	283.10	9.95	162.80	205.90	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{17}H_{36}$	240.47	17	283.80	10.65	294.90	21.75	166.90	212.40	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{19}H_{40}$	268.52	19	295.00	21.85	305.00	31.85	181.00	215.00	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.
$C_{21}H_{44}$	296.58	21	304.40	31.25	312.00	38.85	160.16	216.13	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{23}H_{48}$	324.63	23	312.80	39.65	319.90	46.75	162.95	231.96	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{25}H_{52}$	352.69	25	318.80	45.65	327.40	54.25	166.44	247.53	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{ss} (K)	T_{ss} (°C)	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	$\Delta_{tot}H$ (J g^{-1})	References
$C_{27}H_{56}$	380.74	27	325.00	51.85	331.20	58.05	180.96	258.44	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{29}H_{60}$	409.79	29	330.30	57.15	336.00	62.85	165.45	245.98	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{31}H_{64}$	436.85	31	335.20	62.05	340.00	66.85	167.79	251.57	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{33}H_{68}$	464.90	33	337.90	64.75	343.40	70.25	173.59	255.11	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{35}H_{72}$	492.95	35	344.20	71.05	346.50	73.35	175.27	264.73	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.

Table S3. Thermal properties of alkanes with even number of carbons. The solid-solid transition temperatures (T_{ss}) and melting temperatures (T_{fus}) are listed along with the enthalpies of fusion ($\Delta_{fus}H$) and the total enthalpies of transition ($\Delta_{tot}H = \Delta_{fus}H + \Delta_{ss}H$), when available from the cited references. These data were used in Figs. 2 and 5 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{ss} (K)	T_{ss} (°C)	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	$\Delta_{tot}H$ (J g^{-1})	References
$C_{10}H_{22}$	142.28	10	-	-	243.50	-29.65	-	201.70	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{12}H_{26}$	170.34	12	-	-	263.60	-9.55	-	215.80	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{14}H_{30}$	198.39	14	-	-	279.00	5.85	-	227.00	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{16}H_{34}$	226.44	16	-	-	291.20	18.05	-	235.50	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{18}H_{38}$	254.5	18	-	-	300.20	27.05	-	241.65	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{20}H_{45}$	282.55	20	-	-	310.70	37.55	-	246.00	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.
$C_{22}H_{46}$	310.60	22	315.00	-41.85	316.95	43.80	140.40	234.00	Kahwaji S, Johnson MB, Kheirabadi AC, Groulx D, White MA. A comprehensive study of properties of paraffin phase change materials for solar thermal energy storage and thermal management applications. Energy 2018;162:1169–82. doi:10.1016/j.energy.2018.08.068.
$C_{24}H_{50}$	338.66	24	319.90	-46.75	323.00	49.85	168.90	257.19	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{26}H_{52}$	366.71	26	325.00	-51.85	328.90	55.75	167.43	266.97	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{28}H_{59}$	394.77	28	330.10	-56.95	333.20	60.05	160.85	254.33	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{30}H_{62}$	422.82	30	332.10	-58.95	337.50	64.35	165.08	261.58	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.

Molecular formula	Molecular weight ($g\ mol^{-1}$)	Carbon number	T_{ss} (K)	T_{ss} (°C)	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ ($J\ g^{-1}$)	$\Delta_{tot}H$ ($J\ g^{-1}$)	References
$C_{32}H_{66}$	450.87	32	338.00	-64.85	341.90	68.75	170.78	268.81	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{34}H_{70}$	478.93	34	341.10	-67.95	345.30	72.15	176.43	271.23	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{36}H_{74}$	506.98	36	346.10	-72.95	348.90	75.75	172.99	234.33	Anne-Julie Briard, Mohammed Bouroukba, Dominique Petitjean, Nathalie Hubert and, Dirand* M. Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous n-Alkane Series (C18 to C38 and C41, C44, C46, C50, C54, and C60). J Chem Eng Data 2003;48:497–513. doi:10.1021/JE0201368.
$C_{40}H_{82}$	563.08	40	353.50	-80.35	354.00	80.85	240.70	265.60	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{44}H_{90}$	619.19	44	357.70	-84.55	358.75	85.60	241.70	271.10	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.
$C_{46}H_{94}$	647.24	46	-	273.15	360.70	87.55	-	272.00	Dirand M, Bouroukba M, Briard A-J, Chevallier V, Petitjean D, Corriou J-P. Temperatures and enthalpies of (solid + solid) and (solid + liquid) transitions of n-alkanes. J Chem Thermodyn 2002;34:1255–77. doi:10.1006/jcht.2002.0978.

Table S4. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of fatty alcohols with carbon numbers between 13 and 26. For compounds with more than one data source, the average value of $\Delta_{fus}H$ was calculated. These data were used Figs.1 and 6 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{13}H_{28}O$	200.361	13	1-tridecanol	303.500	30.350	116.29	120.21	J. C. Van Miltenburg, G. J. K. van den Berg, and M. Ramirez, J. Chem. Eng. Data 48, 36 (2003). https://doi.org/10.1021/je025524o
$C_{13}H_{28}O$	200.361	13		318.300	45.150	124.13		V. M. Egorov, V. A. Marikhin, and L. P. Myasnikova, Phys. Solid State 50, 126 (2008). https://doi.org/10.1134/S106378340801023X
$C_{14}H_{30}O$	214.387	14	1-tetradecanol	310.800	37.650	117.08	118.94	T. M. T. Carvalho, L. M. P. F. Amaral, V. M. F. Morais, and M. D. M. C. Ribeiro da Silva, J. Chem. Thermodyn. 85, 129 (2015). https://doi.org/10.1016/j.jct.2015.01.012
$C_{14}H_{30}O$	214.387	14		311.200	38.050	120.81		N. D. D. Carareto, T. Castagnaro, M. C. Costa, and A. J. A. Meirelles, J. Chem. Thermodyn. 78, 99 (2014). https://doi.org/10.1016/j.jct.2014.06.011
$C_{15}H_{32}O$	228.414	15	1-pentadecanol	316.400	43.250	129.59	131.23	L. Ventola, T. Calvet, M. A. Cuevas-Diarte, M. Ramirez, H. A. J. Oonk, D. Mondieig, and P. Negrier, Phys. Chem. Chem. Phys. 6, 1786 (2004). https://doi.org/10.1039/B313106H
$C_{15}H_{32}O$	228.414	15		316.900	43.750	132.87		J. C. Van Miltenburg, G. J. K. van den Berg, and M. Ramirez, J. Chem. Eng. Data 48, 36 (2003). https://doi.org/10.1021/je025524o
$C_{16}H_{34}O$	242.441	16	1-hexadecanol	321.600	48.450	136.53	138.48	N. D. D. Carareto, T. Castagnaro, M. C. Costa, and A. J. A. Meirelles, J. Chem. Thermodyn. 78, 99 (2014). https://doi.org/10.1016/j.jct.2014.06.011
$C_{16}H_{34}O$	242.441	16		322.000	48.850	127.04		T. M. T. Carvalho, L. M. P. F. Amaral, V. M. F. Morais, and M. D. M. C. Ribeiro da Silva, J. Chem. Thermodyn. 97, 70 (2016). https://doi.org/10.1016/j.jct.2016.01.006
$C_{16}H_{34}O$	242.441	16		322.300	49.150	138.59		J. Xing, Z.-C. Tan, Q. Shi, B. Tong, S.-X. Wang, and Y.-S. Li, J. Therm. Anal. Calorim. 92, 375 (2008). https://doi.org/10.1007/s10973-007-8955-1
$C_{16}H_{34}O$	242.441	16		322.900	49.750	140.12		V. Metivaud, A. Lefevre, L. Ventola, P. Negrier, E. Moreno, T. Calvet, D. Mondieig, and M. A. Cuevas-Diarte, Chem. Mater. 17, 3302 (2005). https://doi.org/10.1021/cm050130c
$C_{16}H_{34}O$	242.441	16		323.300	50.150	150.14		L. Ventola, T. Calvet, M. A. Cuevas-Diarte, M. Ramirez, H. A. J. Oonk, D. Mondieig, and P. Negrier, Phys. Chem. Chem. Phys. 6, 1786 (2004). https://doi.org/10.1039/B313106H
$C_{17}H_{36}O$	256.467	17	1-heptadecanol	326.600	53.450	144.27	144.27	J. C. Van Miltenburg, G. J. K. van den Berg, and M. Ramirez, J. Chem. Eng. Data 48, 36 (2003). https://doi.org/10.1021/je025524o
$C_{18}H_{38}O$	270.494	18	1-octadecanol	330.100	56.950	148.25	148.62	N. D. D. Carareto, T. Castagnaro, M. C. Costa, and A. J. A. Meirelles, J. Chem. Thermodyn. 78, 99 (2014). https://doi.org/10.1016/j.jct.2014.06.011
$C_{18}H_{38}O$	270.494	18		331.600	58.450	148.99		G. J. Maximo, N. D. D. Carareto, M. C. Costa, A. O. dos Santos, L. P. Cardoso, M. A. Krahenbuhl, and A. J. A. Meirelles, Fluid Phase Equilib. 366, 88 (2014). https://doi.org/10.1016/j.fluid.2014.01.004
$C_{19}H_{40}O$	284.520	19	1-nonadecanol	333.900	60.750	152.19	152.19	L. Ventola, T. Calvet, M. A. Cuevas-Diarte, M. Ramirez, H. A. J. Oonk, D. Mondieig, and P. Negrier, Phys. Chem. Chem. Phys. 6, 1786 (2004). https://doi.org/10.1039/B313106H
$C_{20}H_{42}O$	298.547	20	1-eicosanol	336.600	63.450	146.04	146.04	G. Nichols, S. Kweskin, M. Frericks, S. Reiter, G. Wang, J. Orf, B. Carvallo, D. Hillesheim, and J. S. Chickos, J. Chem. Eng. Data 51, 475 (2006). https://doi.org/10.1021/je0503857
$C_{22}H_{46}O$	326.600	22	1-docosanol	345.200	72.050	142.59	142.59	B. Tong, Z.-C. Tan, and S.-X. Wang, Wuli Huaxue Xuebao 24, 1699 (2008)

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{26}H_{54}O$	382.706	26	1-hexacosanol	351.700	78.550	177.11	177.11	G. Nichols, S. Kweskin, M. Frericks, S. Reiter, G. Wang, J. Orf, B. Carvallo, D. Hillesheim, and J. S. Chickos, J. Chem. Eng. Data 51, 475 (2006). https://doi.org/10.1021/je0503857

Table S5. Melting temperatures (T_{fus}) and total enthalpies of transition ($\Delta_{tot}H$) of fatty alcohols with carbon numbers between 12 and 26. $\Delta_{tot}H$ is the sum of the enthalpy of solid-solid transition and enthalpy of fusion. These data were used in Fig. 6 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	$\Delta_{tot}H$ (J g^{-1})	References
$C_{12}H_{26}O$	186.334	12	297.53	24.38	206.40	V. M. Egorov, V. A. Marikhin, and L. P. Myasnikova, Phys. Solid State 50, 126 (2008). https://doi.org/10.1134/S106378340801023X
$C_{13}H_{28}O$	200.361	13	304.7	31.55	223.50	J. C. Van Miltenburg, G. J. K. van den Berg, and M. Ramirez, J. Chem. Eng. Data 48, 36 (2003). https://doi.org/10.1021/je025524o
$C_{14}H_{30}O$	214.387	14	311.2	38.05	219.27	J. L. Zeng, Z. Cao, D. W. Yang, F. Xu, L. X. Sun, L. Zhang, and X. F. Zhang, J. Therm. Anal. Calorim. 95, 501 (2009). https://doi.org/10.1007/s10973-008-9274-x
$C_{15}H_{32}O$	228.414	15	316.6	43.45	239.61	C. Mosselman and J. Mouric, J. Chem. Thermodyn. 6, 477–489 (1974). https://doi.org/10.1016/0021-9614(74)90009-3
$C_{16}H_{34}O$	242.441	16	322.2	49.05	240.92	Y. Kakiuchi, T. Sakurai, and T. Suzuki, J. Phys. Soc. Jpn. 5, 369 (1950). https://doi.org/10.1143/JPSJ.5.369
$C_{17}H_{36}O$	256.467	17	325.3	52.15	247.20	G. Nichols, S. Kweskin, M. Frericks, S. Reiter, G. Wang, J. Orf, B. Carvallo, D. Hillesheim, and J. S. Chickos, J. Chem. Eng. Data 51, 475 (2006). https://doi.org/10.1021/je0503857
$C_{18}H_{38}O$	270.494	18	331.2	58.05	246.48	J. C. van Miltenburg, H. A. J. Oonk, and L. Ventola, J. Chem. Eng. Data 46, 90 (2001). https://doi.org/10.1021/je000048s
$C_{19}H_{40}O$	284.520	19	334.5	61.35	254.53	J. C. van Miltenburg, H. A. J. Oonk, and L. Ventola, J. Chem. Eng. Data 46, 90 (2001). https://doi.org/10.1021/je000048s
$C_{20}H_{42}O$	298.547	20	337	63.85	262.61	J. C. van Miltenburg, H. A. J. Oonk, and L. Ventola, J. Chem. Eng. Data 46, 90 (2001). https://doi.org/10.1021/je000048s
$C_{22}H_{46}O$	326.600	22	344.5	71.35	253.52	G. Nichols, S. Kweskin, M. Frericks, S. Reiter, G. Wang, J. Orf, B. Carvallo, D. Hillesheim, and J. S. Chickos, J. Chem. Eng. Data 51, 475 (2006). https://doi.org/10.1021/je0503857
$C_{26}H_{54}O$	382.706	26	353.1	79.95	271.23	A. A. Trapeznikov and T. A. Lomonosova, Zh. Fiz. Khim. 44, 2121–2128 (1970)

Table S6. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of fatty acids with carbon numbers between 11 and 26. These data were used in Fig.1 and Fig. 7 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	References
$C_{11}H_{22}O_2$	186.291	11	301.6	28.45	139.4591	W. E. Garner and F. C. Randall, J. Chem. Soc., Trans. 125, 881 (1924). https://doi.org/10.1039/CT9242500881
$C_{12}H_{24}O_2$	200.318	12	316.6	43.45	180.2137	M. C. Costa, M. Sardo, M. P. Rolemberg, J. A. P. Coutinho, A. J. R. Meirelles, P. Ribeiro-Claro, and M. A. Krahenbuhl, Chem. Phys. Lipids 160, 85 (2009). https://doi.org/10.1016/j.chemphyslip.2009.05.004
$C_{13}H_{26}O_2$	214.344	13	314.5	41.35	154.4244	L. C. Liston, Y. Farnam, M. Krafcik, J. Weiss, K. Erk, and B. Y. Tao, Appl. Therm. Eng. 96, 501 (2016). https://doi.org/10.1016/j.applthermaleng.2015.11.007
$C_{14}H_{28}O_2$	228.371	14	325.9	52.75	185.225	J. Huang, S. Lu, X. Kong, S. Liu, and Y. Li, Materials 6, 4758 (2013). https://doi.org/10.3390/ma6104758
$C_{15}H_{30}O_2$	242.398	15	325.7	52.55	171.2889	J. C. van Miltenburg and H. A. J. Oonk, J. Chem. Eng. Data 50, 1348 (2005). https://doi.org/10.1021/je050065n
$C_{16}H_{32}O_2$	256.424	16	335.4	62.25	210.1987	T. Inoue, Y. Hisatsugu, R. Ishikawa, and M. Suzuki, Chem. Phys. Lipids 127, 161 (2004). https://doi.org/10.1016/j.chemphyslip.2003.10.013
$C_{17}H_{34}O_2$	270.451	17	334.3	61.15	189.7943	J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{18}H_{36}O_2$	284.477	18	342.8	69.65	222.1619	F. O. Cedeno, M. M. Prieto, A. Espina, and J. R. Garcia, Thermochim. Acta 369, 39 (2001). https://doi.org/10.1016/S0040-6031(00)00752-8
$C_{19}H_{38}O_2$	298.504	19	340.4	67.25	190.9523	J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{20}H_{40}O_2$	312.530	20	347.8	74.65	229.0977	J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{21}H_{42}O_2$	326.557	21	346.7	73.55	192.9219	A. Sari, A. Bicer, and A. Karaipekli, Mater. Lett. 63, 1213 (2009). https://doi.org/10.1016/j.matlet.2009.02.045
$C_{22}H_{44}O_2$	340.584	22	353.9	80.75	236.359	V. M. Egorov, V. A. Marikhin, and L. P. Myasnikova, Polym. Sci., Ser. A 53, 906 (2011). https://doi.org/10.1134/S0965545X11100038
$C_{23}H_{46}O_2$	354.610	23	352	78.85	211.4999	J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{24}H_{48}O_2$	368.637	24	356.5	83.35	229.223	J. Wilson, C. Gobble, and J. Chickos, J. Chem. Eng. Data 60, 202 (2015). https://doi.org/10.1021/je5009729
$C_{26}H_{52}O_2$	396.690	26	358.8	85.65	223.0962	A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030

Table S7. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of esters with carbon number between 10 and 38. The data are sorted by ascending carbon numbers. For compounds with more than one data source, the average values of T_{fus} and $\Delta_{fus}H$ were calculated. *A* = number of carbon atoms in the alkyl chain; *B* = number of carbon atoms in the ester root. These data were used in Fig.1, Fig. 3, and Fig. 8 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{10}H_{20}O_2$	172.270	10	5	5	Pentyl valerate	198.65		-74.5		99.100		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{12}H_{24}O_2$	200.318	12	2	10	Ethyl decanoate	253.6	252.80	-19.55	-20.35	161.194	152.10	T. M. T. Carvalho, L. M. P. F. Amaral, V. M. F. Morais, and M. D. M. C. Ribeiro da Silva, J. Chem. Thermodyn. 85, 129 (2015). https://doi.org/10.1016/j.jct.2015.01.012
$C_{12}H_{24}O_2$	200.318	12				252		-21.15		143.000		Noël JA, Kahwaji S, White MA. Molecular Structure and Melting: Implications for Phase. Can J Chem 2017:cjc-2017-0578. https://doi.org/10.1139/cjc-2017-0578
$C_{12}H_{24}O_2$	200.318	12	4	8	Butyl octanoate	230		-43.15		140.000		Noël JA, Kahwaji S, White MA. Molecular Structure and Melting: Implications for Phase. Can J Chem 2017:cjc-2017-0578. https://doi.org/10.1139/cjc-2017-0578
$C_{12}H_{24}O_2$	200.318	12	6	6	Hexyl hexanoate	217		-56.15		108.000		Noël JA, Kahwaji S, White MA. Molecular Structure and Melting: Implications for Phase. Can J Chem 2017:cjc-2017-0578. https://doi.org/10.1139/cjc-2017-0578
$C_{13}H_{26}O_2$	214.344	13	2	11	Ethyl undecanoate	259.2		-13.95		168.701		V. M. Egorov, V. A. Marikhin, and L. P. Myasnikova, Polym. Sci., Ser. A 53, 906 (2011). https://doi.org/10.1134/S0965545X11100038
$C_{14}H_{28}O_2$	228.371	14	2	12	Ethyl dodecanoate	271.5	272.35	-1.65	-0.80	176.905	167.42	G. J. Maximo, N. D. D. Carereto, M. C. Costa, A. O. dos Santos, L. P. Cardoso, M. A. Krahenbuhl, and A. J. A. Meirelles, Fluid Phase Equilib. 366, 88 (2014). https://doi.org/10.1016/j.fluid.2014.01.004
$C_{14}H_{28}O_2$	228.371	14				271.5		-1.65		40.767		M. D. Robustillo, D. F. Barbosa, A. J. de Almeida Meirelles, and P. de Alcantara Pessoa Filho, Fluid Phase Equilib. 361, 188 (2014). https://doi.org/10.1016/j.fluid.2013.10.024
$C_{14}H_{28}O_2$	228.371	14				273.2		0.05		157.945		E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{15}H_{30}O_2$	242.398	15	2	13	Ethyl tridecanoate	272.4		-0.75		167.906		W. E. Acree, Jr., Thermochim. Acta 219, 97 (1993); and references therein. https://doi.org/10.1016/0040-6031(93)80486-T
$C_{15}H_{30}O_2$	242.398	15	1	14	Methyl tetradecanoate (methyl myristate)	293.9	290.88	20.75	17.73	188.616	189.31	E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{15}H_{30}O_2$	242.398	15	1	14		287.85		14.7		190.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069
$C_{16}H_{32}O_2$	256.430	16	2	14	Ethyl myristate	287.25		14.1		173.400		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{16}H_{32}O_2$	256.430	16	4	12	Butyl dodecanoate	268.15		-5		175.400		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{17}H_{34}O_2$	270.451	17	1	16	Methyl hexadecanoate (methyl palmitate)	300.61	303.55	27.46	30.40	188.352	214.68	M. Benziane, K. Khimeche, A. Dahmani, S. Nezar, and D. Trache, J. Therm. Anal. Calorim. 112, 229 (2013). https://doi.org/10.1007/s10973-012-2654-2
$C_{17}H_{34}O_2$	270.451	17				302.2		29.05		231.466		E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{17}H_{34}O_2$	270.451	17				302.2		29.05		214.827		A. M. King and W. E. Garner, J. Chem. Soc. 1936, 1372–1376. https://doi.org/10.1039/jr9360001372
$C_{17}H_{34}O_2$	270.451	17				302.2		29.05		198.927		M. W. Babich, S. W. Hwang, and R. D. Mounts, Thermochim. Acta 210, 83 (1992). https://doi.org/10.1016/0040-6031(92)80279-6
$C_{17}H_{34}O_2$	270.451	17				303.7		30.55		217.119		G. Gbabode, P. Negrier, D. Mondieig, E. M. Calvo, T. Calvet, and M. A. Cuevas-Diarte,

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
												Chem. - Eur. J. 13, 3150 (2007). https://doi.org/10.1002/chem.200600955
$C_{17}H_{34}O_2$	270.451	17				305.1		31.95		207.690		I. Abe, T. Kuroya, and K. Kusano, J. Jpn. Oil Chem. Soc. 34, 681 (1985). https://doi.org/10.5650/jos1956.34.681
$C_{17}H_{34}O_2$	270.451	17				305.2		32.05		207.062		W. E. Acree, Jr., Thermochim. Acta 219, 97 (1993); and references therein. https://doi.org/10.1016/0040-6031(93)80486-T
$C_{17}H_{34}O_2$	270.451	17				307.2		34.05		252.024		G. Berchiesi, M. A. Bercuiesi, G. G. Lobbia, and D. Leonesi, Gazz. Chim. Ital. 106, 549–555 (1976)
$C_{17}H_{34}O_2$	270.451	17	7	10	Heptyl decanoate	269.25		-3.9		147.600		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{18}H_{36}O_2$	284.477	18	1	17	Methyl heptadecanoate	304.2		31.05		169.082		M. D. Robustillo, D. F. Barbosa, A. J. de Almeida Meirelles, and P. de Alcantara Pessoa Filho, Fluid Phase Equilib. 361, 188 (2014). https://doi.org/10.1016/j.fluid.2013.10.024
$C_{19}H_{38}O_2$	298.504	19	1	18	Methyl stearate	308.78		35.63		204.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069
$C_{19}H_{38}O_2$	298.504	19	5	14	Pentyl tetradecanoate	283.05		9.9		177.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{19}H_{38}O_2$	298.504	19	2	17	Ethyl margarate (ethyl heptadecanoate)	298.4		25.25		121.271		M. Benziane, K. Khimeche, A. Dahmani, S. Nezar, and D. Trache, J. Therm. Anal. Calorim. 112, 229 (2013). https://doi.org/10.1007/s10973-012-2654-2
$C_{20}H_{40}O_2$	312.530	20				313.2		40.05		204.140		M. M. Omar, J. Chem. Soc. C 2038–2040 (1967). https://doi.org/10.1039/j39670002038
$C_{20}H_{40}O_2$	312.530	20	1	19	Methyl nonadecanoate	313.2	313.20	40.05	40.05	136.947	170.54	E. Moreno, R. Cordobilla, T. Calvet, M. A. Cuevas-Diarte, G. Gbabode, P. Negrier, D. Mondieig, and H. A. J. Oonk, New J. Chem. 31, 947 (2007). https://doi.org/10.1039/b700551b

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{21}H_{42}O_2$	326.557	21	2	19	Ethyl nonadecanoate	309		35.85		131.983		A. M. King and W. E. Garner, J. Chem. Soc. 1936, 1372–1376. https://doi.org/10.1039/jr9360001372
$C_{21}H_{42}O_2$	326.557	21	1	20	Methyl eicosanoate	319.2	318.53	46.05	45.38	227.525	222.07	G. Gbabode, P. Negrier, D. Mondieig, E. M. Calvo, T. Calvet, and M. A. Cuevas-Diarte, Chem. - Eur. J. 13, 3150 (2007). https://doi.org/10.1002/chem.200600955
$C_{21}H_{42}O_2$	326.557	21				319.2		46.05		225.688		M. M. Omar, J. Chem. Soc. C 2038–2040 (1967). https://doi.org/10.1039/j39670002038
$C_{21}H_{42}O_2$	326.557	21				317.2		44.05		213.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{21}H_{42}O_2$	326.557	21	5	16	Ppentyl hexadecanoate	292.75		19.6		187.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{22}H_{44}O_2$	340.584	22	6	16	Hexylhexadecanoate	287.6		14.45		164.982		M. M. Omar, J. Chem. Soc. C 2038–2040 (1967). https://doi.org/10.1039/j39670002038
$C_{22}H_{44}O_2$	340.584	22	10	12	Decyldodecanoate	293.2		20.05		186.944		A. M. King and W. E. Garner, J. Chem. Soc. 1934, 1449. https://doi.org/10.1039/jr9340001449
$C_{22}H_{44}O_2$	340.584	22	2	20	Ethyleicosanoate	313.6	314.30	40.45	41.15	201.419	201.45	J. E. Baldvins and R. G. Weiss, Liq. Cryst. 26, 897 (1999). https://doi.org/10.1080/026782999204598
$C_{22}H_{44}O_2$	340.584	22				315		41.85		201.478		J. E. Baldvins and R. G. Weiss, Liq. Cryst. 26, 897 (1999). https://doi.org/10.1080/026782999204598
$C_{22}H_{44}O_2$	340.584	22	1	21	Methyl heneicosanoate	321.2		48.05		220.504		J. A. Wilson and J. S. Chickos, J. Chem. Eng. Data 58, 322 (2013). https://doi.org/10.1021/je300902c
$C_{23}H_{46}O_2$	354.610	23	1	22	Methyl docosanoate (methyl behenate)	327.2	325.15	54.05	52.00	235.470	222.52	G. Gbabode, P. Negrier, D. Mondieig, E. M. Calvo, T. Calvet, and M. A. Cuevas-Diarte, Chem. - Eur. J. 13, 3150 (2007). https://doi.org/10.1002/chem.200600955
$C_{23}H_{46}O_2$	354.610	23				327.2		54.05		232.086		A. M. King and W. E. Garner, J. Chem. Soc. 1936, 1372–1376. https://doi.org/10.1039/jr9360001372
$C_{23}H_{46}O_2$	354.610	23				321.05		47.9		200.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
												2018;8:1069. https://doi.org/10.3390/APP8071069
$C_{23}H_{46}O_2$	354.610	23	5	18	Pentyl octadecanoate	298.32		25.17		151.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{24}H_{48}O_2$	368.637	24	2	22		321	321.00	47.85	47.85	211.102	176.08	E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{24}H_{48}O_2$	368.637	24				321		47.85		141.060		M. M. Omar, J. Chem. Soc. C 2038–2040 (1967). https://doi.org/10.1039/j39670002038
$C_{24}H_{48}O_2$	368.637	24	10	14		298.35		25.2		196.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069.
$C_{25}H_{50}O_2$	382.663	25	2	23	Ethyl tricosanoate	326		52.85		149.792		J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{25}H_{50}O_2$	382.663	25	1	24	Methyl tetracosanoate	331.2		58.05		235.194		M. M. Omar, J. Chem. Soc. C 2038–2040 (1967). https://doi.org/10.1039/j39670002038
$C_{25}H_{50}O_2$	382.663	25	5	20	Pentyl eicosanoate	308.6		35.45		189.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{26}H_{52}O_2$	396.690	26	16	10	Hexadecyl decanoate	302.6		29.45		186.292		E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{26}H_{52}O_2$	396.690	26	14	12	Tetradecyl dodecanoate	311.3		38.15		207.971		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{26}H_{52}O_2$	396.690	26	1	15	Methyl pentacosanoate	332.2		59.05		231.919		J. Wilson, C. Gobble, and J. Chickos, J. Chem. Eng. Data 60, 202 (2015). https://doi.org/10.1021/je5009729
$C_{26}H_{52}O_2$	396.690	26	10	16		302.18		29.03		193.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{27}H_{54}O_2$	410.716	27	14	13	Tetradecyl tridecanoate	313.2		40.05		207.881		J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{27}H_{54}O_2$	410.716	27	1	26	Methyl hexacosanoate	336.2		63.05		246.642		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{27}H_{54}O_2$	410.716	27	5	22	Pentyl docosanoate	315.53		42.38		165.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{28}H_{56}O_2$	424.743	28	16	18	Hexadecyl dodecanoate	311.4		38.25		195.412		E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{28}H_{56}O_2$	424.743	28	14	14	Tetradecyl tetradecanoate	314.8	316.23	41.65	43.08	210.480	202.14	A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{28}H_{56}O_2$	424.743	28				317.65		44.5		193.800		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{28}H_{56}O_2$	424.743	28	1	27	Methyl heptacosanoate	336.2		63.05		237.085		A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030
$C_{28}H_{56}O_2$	424.743	28	10	18		309.37		36.22		192.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069
$C_{29}H_{58}O_2$	438.770	29	14	15	Tetradecyl pentadecanoate	318.6		45.45		214.805		J. S. Chickos and W. J. Hanshaw, Chem. Eng. Data 49, 77 (2004). https://doi.org/10.1021/je0301747
$C_{29}H_{58}O_2$	438.770	29	1	18	Methyl octacosanoate	340.2		67.05		250.017		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{30}H_{60}O_2$	452.796	30	18	12	Octadecyl dodecanoate	315.4		42.25		201.040		A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030
$C_{30}H_{60}O_2$	452.796	30	14	16	Tetradecyl hexadecanoate	321.2		48.05		213.783		A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{30}H_{60}O_2$	452.796	30	16	14	Hexadecyl tetradecanoate	322.6		49.45		225.267		A. A. Aydin, Sol. Energy Mater. Sol. Cells 113, 44 (2013). https://doi.org/10.1016/j.solmat.2013.01.024
$C_{30}H_{60}O_2$	452.796	30	10	20	Decyl eicosanoate	314.04		40.89		232.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Analysis of bio-based fatty esters PCM's thermal properties and investigation of trends in relation to chemical structures. Appl Sci 2019;9:225. https://doi.org/10.3390/app9020225
$C_{30}H_{60}O_2$	452.796	30	12	18	Lauryl stearate	318.85		45.7		185.700		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{31}H_{62}O_2$	466.823	31	14	17	Tetradecyl heptadecanoate	319.9		46.75		217.192		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{32}H_{64}O_2$	480.849	32	18	14	Octadedcyl tetradecanoate	322.1		48.95		203.536		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015
$C_{32}H_{64}O_2$	480.849	32	14	18	Tetradecyl octadecanoate	322.8		49.65		221.899		A. A. Aydin, Sol. Energy Mater. Sol. Cells 113, 44 (2013). https://doi.org/10.1016/j.solmat.2013.01.024
$C_{32}H_{64}O_2$	480.849	32	16	16	Hexadecyl hexadecanoate	324.4	325.93	51.25	52.78	217.532	218.22	A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030
$C_{32}H_{64}O_2$	480.849	32				327.45		54.3		218.900		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{32}H_{64}O_2$	480.849	32	2	30	Ethyl triacontanoate	341.5		68.35		155.974		E. S. Domalski and E. D. Hearing, J. Phys. Chem. Ref. Data 25, 1 (1996), and references therein. https://doi.org/10.1063/1.555985
$C_{32}H_{64}O_2$	480.849	32	10	22		317.95		44.8		193.000		Ravotti R, Fellmann O, Lardon N, Fischer LJ, Stamatiou A, Worlitschek J. Synthesis and Investigation of Thermal Properties of Highly Pure Carboxylic Fatty Esters to Be Used as PCM. Appl Sci 2018, Vol 8, Page 1069 2018;8:1069. https://doi.org/10.3390/APP8071069
$C_{33}H_{66}O_2$	494.876	33	14	19	Tetradecyl nonadecanoate	323.4		50.25		203.223		A. A. Aydin and H. Okutan, Sol. Energy Mater. Sol. Cells 95, 2752 (2011). https://doi.org/10.1016/j.solmat.2011.04.015

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	A	B	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_{34}H_{68}O_2$	508.903	34	16	18	Hexadecyl octadecanoate	327.8		54.65		214.186		A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030
$C_{34}H_{68}O_2$	508.903	34	18	16	Octadecyl hexadecanoate	330.5		57.35		219.747		A. A. Aydin, Sol. Energy Mater. Sol. Cells 113, 44 (2013). https://doi.org/10.1016/j.solmat.2013.01.024
$C_{34}H_{68}O_2$	508.903	34	12	22	Lauryl behenate	327.65		54.5		185.200		Stamatiou A, Obermeyer M, Fischer LJ, Schuetz P, Worlitschek J. Investigation of unbranched, saturated, carboxylic esters as phase change materials. Renew Energy 2017;108:401–9. https://doi.org/10.1016/j.renene.2017.02.056
$C_{36}H_{72}O_2$	536.956	36	18	18	Octadecyl octadecanoate	332.4		59.25		214.934		A. A. Aydin, Sol. Energy Mater. Sol. Cells 104, 102 (2012). https://doi.org/10.1016/j.solmat.2012.04.030
$C_{36}H_{72}O_2$	536.956	36	16	20	Hexadecyl eicosanoate	332.5		59.35		226.462		A. A. Aydin, Sol. Energy Mater. Sol. Cells 113, 44 (2013). https://doi.org/10.1016/j.solmat.2013.01.024
$C_{38}H_{76}O_2$	565.009	38	18	20	Octadecyl eicosanoate	338.1		64.95		226.120		A. A. Aydin, Sol. Energy Mater. Sol. Cells 113, 44 (2013). https://doi.org/10.1016/j.solmat.2013.01.024

Table S8. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of diamides. These data were used in Fig.1 and Fig. 9 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	References
$C_8H_{16}N_2O_2$	172.228	8	Suberamide	493.23	220.08	338.9112	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004
$C_9H_{18}N_2O_2$	186.254	9	Azelamide	450.41	177.26	295.4031	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004
$C_{10}H_{20}N_2O_2$	200.28	10	Sebacamide	484.31	211.16	343.2694	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004
$C_{11}H_{22}N_2O_2$	214.305	11	Undecandiamide	451.2	178.05	300.5069	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004
$C_{12}H_{24}N_2O_2$	228.331	12	Dodecandiamide	466.1	192.95	322.7768	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004
$C_{14}H_{28}N_2O_2$	256.384	14	Tetradecandiamide	469.3	196.15	302.0856	E. Badea, G. Della Gata, D. D. Angelo, B. Brunetti, and Z. Reckova, J. Chem. Thermodyn. 38, 1546 (2006). https://doi.org/10.1016/j.jct.2006.04.004

Table S9. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of diamines. For compounds with more than one data source, the average values of T_{fus} and $\Delta_{fus}H$ were calculated. These data were used in Fig.1 and Fig. 9 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	Average T_{fus} (K)	T_{fus} (°C)	Average T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	Average $\Delta_{fus}H$ (J g^{-1})	References
$C_8H_{20}N_2$	144.26	8	Octane-1,8-diamine	324.790	324.790	51.640	51.640	353.390	353.390	L. Dall'acqua, G. Della Gatta, B. Nowicka, and P. Ferloni, J. Chem. Thermodyn. 34, 1 (2002). https://doi.org/10.1006/jcht.2001.0950
$C_9H_{22}N_2$	158.286	9	Nonane-1,9-diamine	308.120	308.120	34.970	34.970	228.953	228.953	L. Dall'acqua, G. Della Gatta, B. Nowicka, and P. Ferloni, J. Chem. Thermodyn. 34, 1 (2002). https://doi.org/10.1006/jcht.2001.0950
$C_{10}H_{24}N_2$	172.312	10	Decane-1,10-diamine	332.880	332.880	59.730	59.730	335.496	335.496	L. Dall'acqua, G. Della Gatta, B. Nowicka, and P. Ferloni, J. Chem. Thermodyn. 34, 1 (2002). https://doi.org/10.1006/jcht.2001.0950
$C_{11}H_{26}N_2$	186.338	11	Undecane-1,11-diamine	313.640	313.640	40.490	40.490	258.026	258.026	L. Dall'acqua, G. Della Gatta, B. Nowicka, and P. Ferloni, J. Chem. Thermodyn. 34, 1 (2002). https://doi.org/10.1006/jcht.2001.0950
$C_{12}H_{28}N_2$	200.364	12	1,12-dodecanediamine	340.500	341.150	67.350	68.000	334.890	334.890	L. Dall'acqua, G. Della Gatta, B. Nowicka, and P. Ferloni, J. Chem. Thermodyn. 34, 1 (2002). https://doi.org/10.1006/jcht.2001.0950
$C_{12}H_{28}N_2$	200.364	12	1,12-dodecanediamine	341.800		68.650		334.890		K. Khimeche, Y. Boumrah, M. Benziane, and A. Dahmani, Thermochim. Acta 444, 166 (2006). https://doi.org/10.1016/j.tca.2006.03.011

Table S10. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of dinitriles. These data were used in Fig.1 and Fig. 9 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	References
$C_{10}H_{16}N_2$	164.248	10	Sebaconitrile	281.180	8.030	171.509	Badea E, Blanco I, Della Gatta G. Fusion and solid-to-solid transitions of a homologous series of alkane-α,ω-dinitriles. J Chem Thermodyn 2007;39:1392–8. https://doi.org/10.1016/J.JCT.2007.03.005
$C_{11}H_{18}N_2$	178.277	11	Undecanonitrile	266.140	-7.010	145.897	Badea E, Blanco I, Della Gatta G. Fusion and solid-to-solid transitions of a homologous series of alkane-α,ω-dinitriles. J Chem Thermodyn 2007;39:1392–8. https://doi.org/10.1016/J.JCT.2007.03.005
$C_{12}H_{20}N_2$	192.304	12	Dodecanedinitrile	294.230	21.080	178.519	Badea E, Blanco I, Della Gatta G. Fusion and solid-to-solid transitions of a homologous series of alkane-α,ω-dinitriles. J Chem Thermodyn 2007;39:1392–8. https://doi.org/10.1016/J.JCT.2007.03.005
$C_{14}H_{24}N_2$	220.358	14	Tetradecaneditrile	309.550	36.400	182.294	Badea E, Blanco I, Della Gatta G. Fusion and solid-to-solid transitions of a homologous series of alkane-α,ω-dinitriles. J Chem Thermodyn 2007;39:1392–8. https://doi.org/10.1016/J.JCT.2007.03.005

Table S11. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of diols. For compounds with carbon number ≥ 17, $\Delta_{fus}H$ data were not available from the cited references. These data were used in Fig.1 and Fig. 9 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	References
$C_{10}H_{22}O_2$	174.276	10	1,10-decanediol	345.800	72.650	258.211	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{11}H_{24}O_2$	188.302	11	1,11-undecanediol	334.100	60.950	243.757	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{12}H_{26}O_2$	202.328	12	1,12-dodecanediol	352.900	79.750	267.882	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{13}H_{28}O_2$	216.354	13	1,13-tridecanediol	350.300	77.150	253.289	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{14}H_{30}O_2$	230.38	14	1,14-tetradecanediol	359.200	86.050	275.632	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{15}H_{32}O_2$	244.406	15	1,15-pentadecanediol	361.200	88.050	267.178	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{16}H_{34}O_2$	258.432	16	1,16-hexadecanediol	366.000	92.850	281.699	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{17}H_{36}O_2$	272.458	17	1,17-heptadecanediol	367.300	94.150	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{18}H_{38}O_2$	286.484	18	1,18-octadecanediol	371.500	98.350	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{19}H_{40}O_2$	300.51	19	1,19-nonadecanediol	373.900	100.750	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{20}H_{42}O_2$	314.536	20	1,20-eicosanediol	376.100	102.950	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125

Table S12. Melting temperatures (T_{fus}) and enthalpies of fusion ($\Delta_{fus}H$) of dioic acids. For compounds with carbon numbers 16 and 18, $\Delta_{fus}H$ data were not available from the cited references. These data were used in Fig.1 and Fig. 9 in the manuscript.

Molecular formula	Molecular weight (g mol^{-1})	Carbon number	Compound name	T_{fus} (K)	T_{fus} (°C)	$\Delta_{fus}H$ (J g^{-1})	References
$C_{10}H_{18}O_4$	202.244	10	Decanedioic acid	404.000	130.850	201.737	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{11}H_{20}O_4$	216.27	11	Undecanedioic acid	385.000	111.850	183.567	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{12}H_{22}O_4$	230.296	12	Dodecanedioic acid	402.500	129.350	219.717	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{13}H_{24}O_4$	244.322	13	Tridecanedioic acid	386.300	113.150	202.192	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{14}H_{26}O_4$	258.348	14	Tetradecanedioic acid	397.300	124.150	218.697	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{16}H_{30}O_4$	286.41	16	Hexadecanedioic acid	395.400	122.250	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125
$C_{18}H_{34}O_4$	314.5	18	Octadecanedioic acid	398.100	124.950	-	Costa JCS, Santos LMNBF. Chain-Length Dependence of the Thermodynamic Behavior of Homologous α,ω-Disubstituted Alkanes. J Chem Eng Data 2019;64:2229–46. https://doi.org/10.1021/ACS.JCED.9B00125