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A Thermodynamic Investigation of Tripalmitin. Molar Heat Capacities of the α- and *β*-form between 10 K and 350 K

Johannes C. van Miltenburg*,† and Erik ten Grotenhuis‡

Chemical Thermodynamics Group, Debye Institute, Utrecht University, Padualaan 8,
3584 CH Utrecht, The Netherlands, and Netherlands Institute for Dairy Research (NIZO),
P.O. Box 20, 6710 BA Ede, The Netherlands

Molar heat capacities of two forms of tripalmitin (the α- and the *β*-forms) were measured between 10 K and 350 K. The enthalpy of fusion of the metastable α-form was calculated to be 108.4 $\mathrm{kJ{\cdot}mol^{-1}}$ at a melting point of 318 K, according to differential scanning calorimetry measurements. For the stable *β*-form a value of 177.2 $\mathrm{kJ{\cdot}mol^{-1}}$ was found at the melting temperature of 339.01 K. To get a consistent set of Gibbs energy values a zero entropy of (18 ± 2) $\mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$ has to be assumed for the α-phase. The molar heat capacity of the liquid phase was represented by $C_\mathrm{p} = \{1100.15 + 1.866{\cdot}T/\mathrm{K}\}\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$.

Introduction

Triglycerides are the main constituents of fats and oils. They are composed of three fatty acids esterified to a glycerol backbone in the *sn*-1, *sn*-2, and *sn*-3 positions. The fatty acids can be saturated or unsaturated and can vary in their lengths. The lengths of the fatty acid chains, their degree of unsaturation, and the asymmetry of the triglyceride molecule determine the thermal properties, of which the melting point stands out. (D′Souza et al.,1990; Small, 1986).

Each natural fat or oil is characterized by its specific complex composition. Relatively more unsaturated fatty acids are found in vegetable fats or oil than in animal fats or oil. For example, in cocoa butter the most common triglyceride is palmitic−oleic−palmitic glyceride. Milk fat consists mostly of triglycerides such as palmitic−palmitic−butyric glyceride. Although fats and oils differ to a considerable extent in their composition, they possess the same general phase behavior. In the solid state, triglycerides can occur in various polymorphic crystalline forms. The three most commonly encountered forms are the α-form, the *β*′-form, and the *β*-form. The *β*-form is the most stable form, and triclinic subcells build up its unit cell. The *β*′-form is less stable than the *β*-form. However, some highly asymmetrical triglycerides and complex mixtures of triglycerides could be stable in the *β*′-form and never transform to *β*-crystals. It is generally assumed that the *β*′-form has an orthogonal unit cell. The α-form is the least stable form in which the fatty acid chains form a hexagonal lattice in which they can rotate with a high degree of freedom. Although the phase behavior of the pure triglycerides and natural fats and oils (which are mixtures of many triglycerides) differ in certain details, the general phase behavior is similar. For this reason many experiments have been performed on pure triglycerides, for example tripalmitin.

In this work the molar heat capacities of α-tripalmitin and *β*-tripalmitin are reported, starting at temperatures as low as 5 K. In addition, the enthalpy of transition between the two crystal forms was measured.

Experimental Section

Tripalmitin was purchased from Fluka AG, with a reported purity of >99%. A mass of 5.21 g was enclosed in the calorimeter vessel. After evacuation, about 1000 Pa of helium gas was admitted to enhance the heat exchange within the vessel. The calorimeter and the measuring procedure have been described previously (van Miltenburg et al., 1987; 1998). Temperatures were measured with a calibrated rhodium−iron thermometer (25 Ohm at 273 K, calibrated by Oxford Instruments against the IPTS-68 and corrected to the ITS-90) and an AC-bridge (Tinsley Senator, Tinsley and Co, UK). The measuring procedure consists of alternating stabilization periods and heat input periods. The length of these periods depends on the temperature region. Below 30 K, periods of about 200 s are used; above this temperature the stabilization periods vary between 400 and 800 s. The surroundings of the calorimeter vessel consist of two regulated shields and a wire heater. The temperature differences between these shields and the vessel are regulated to within 0.001 K.

In the first experiment the compound was heated to a temperature above the melting point. Then, cooling the melt at a cooling rate of 4 $\mathrm{K{\cdot}min^{-1}}$ resulted in a metastable crystal form, which started to transform to a more stable state during heating at about 305 K. This transformation was accompanied by a large evolved heat, which raised the temperature of the vessel about 17 K. From published differential scanning calorimetry (DSC) measurements (Kellens et al., 1992) it is known that the α-form of tripalmitin melts at about 318 K. Because the spontaneous temperature rise resulted in a considerably higher temperature, it must be assumed that during this crystallization process a liquid was formed that further transformed to a more stable solid form. This might be the *β*′-form, intermediate between the α-form and the stable *β*-form. After the large exothermic effect a smaller exothermic effect was found, which persisted up to the melting point of the *β*-form at 339.03 K. In the next experiment the sample was melted and cooled as before, then was heated to 310 K.

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* To whom correspondence should be addressed. Fax: +31 302533946. E-mail: miltenb@chem.uu.nl.

† Utrecht University.

‡ Netherlands Institute for Dairy Research.

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Table 1. Experimental Heat Capacity Data and Enthalpy Values of β-Tripalmitin

T (K)	C_p ($J \cdot K^{-1} \cdot mol^{-1}$)	ΔH ($J \cdot mol^{-1}$)	T (K)	C_p ($J \cdot K^{-1} \cdot mol^{-1}$)	ΔH ($J \cdot mol^{-1}$)	T (K)	C_p ($J \cdot K^{-1} \cdot mol^{-1}$)	ΔH ($J \cdot mol^{-1}$)
6.97	4.42	0.38	83.13	478.24	18530	252.15	1076.2	149354
8.16	6.62	6.66	85.96	490.73	19898	256.08	1090.3	153611
9.04	9.23	14.34	88.79	502.81	21304	260.01	1108.8	157931
9.64	11.34	21.42	91.63	514.31	22750	263.93	1126.7	162317
10.70	14.60	33.53	94.49	525.91	24234	267.85	1145.2	166767
11.43	17.54	46.98	97.35	537.22	25755	271.77	1164.3	171293
12.41	21.18	64.33	100.22	547.01	27312	275.69	1184.9	175896
13.19	24.93	84.57	104.53	563.34	29707	279.61	1205.9	180579
14.31	29.94	113	109.55	581.14	32576	283.52	1229.1	185345
15.13	34.19	142	114.43	597.71	35456	287.43	1252.8	190198
16.35	40.64	185	119.19	614.57	38339	291.34	1279.3	195141
17.18	45.43	225	123.83	630.74	41229	295.23	1306.5	200180
18.48	52.98	285	128.37	646.05	44127	299.13	1334.1	205328
19.35	58.28	337	132.82	660.72	47033	303.03	1362.1	210581
20.70	66.69	419	137.19	674.99	49948	306.92	1391.8	215944
21.61	73.13	486	141.47	689.36	52869	310.79	1418.5	221386
23.01	82.94	592	145.68	702.92	55797	314.63	1448.6	226878
23.95	89.98	677	149.84	701.77	58720	318.41	1480.9	232425
25.39	101.17	812	153.94	727.76	61652	322.15	1517.3	238032
26.37	108.24	918	157.97	742.56	64618	325.84	1560.8	243708
27.89	117.60	1086	161.96	754.81	67600	329.47	1624.2	249483
28.92	125.14	1216	165.89	766.79	70594	332.96	1803.8	255463
30.51	137.27	1421	169.81	779.28	73620	335.88	3079	262280
33.20	160.07	1820	173.72	791.58	76692	337.47	13439	271027
35.16	175.64	2150	177.63	804.28	79813	337.99	34235	281327
36.34	185.07	2362	181.55	817.21	82988	338.24	59419	292039
38.23	197.10	2736	185.46	829.94	86213	338.39	88202	302887
40.78	216.94	3262	189.38	842.46	89489	338.50	120338	313801
43.24	235.85	3817	193.30	855.21	92816	338.58	155580	324756
45.69	254.63	4419	197.22	868.54	96195	338.64	195027	335735
48.19	273.15	5078	201.15	881.70	99629	338.69	240283	346729
50.71	291.72	5793	205.07	894.87	103111	338.74	295129	357737
53.28	309.98	6564	208.99	908.49	106647	338.77	385697	368761
55.87	328.30	7391	212.91	922.28	110240	338.79	519967	379796
58.49	345.52	8275	216.84	936.36	113885	338.81	887933	390842
61.14	362.08	9213	220.76	950.66	117588	338.82	2418158	401898
63.82	378.72	10205	224.69	965.41	121351	338.83	703727	412953
66.51	394.44	11247	228.61	980.39	125169	338.87	153355	423958
69.23	409.67	12341	232.54	995.78	129044	340.22	2746.7	433054
71.98	424.43	13487	236.46	1011.27	132983	343.27	1741.5	439677
74.74	438.74	14679	240.39	1027.09	136985	346.72	1747.4	445697
77.52	452.56	15918	244.31	1043.22	141045	350.16	1751.3	451724
80.32	465.60	17202	248.23	1059.70	145165			

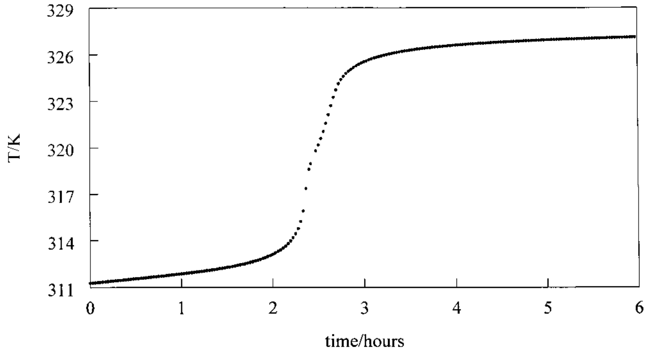

Figure 1. Spontaneous temperature changes under adiabatic conditions during the recrystallization of the metastable α-form to the stable β-form.

The spontaneous temperature rise was followed without supplying energy to the vessel. Adiabatic conditions were maintained throughout the experiment. In Figure 1 the temperature−time curve is given. The recrystallization rate increased up to the melting point temperature of the α-form. The second part of this curve corresponds to the transformation of the liquid to the β or the β'-form. It is also clear from this curve that even after 6 h the transformation was not complete. So, to prepare the stable β-form in the calorimeter, the procedure had to be repeated. This time, after the spontaneous crystallization, the sample was heated to a temperature below the melting point of the β-form (339 K) and held overnight. Then the sample was cooled slowly. For the measurement of the α-form, the compound was cooled as rapidly as the apparatus would allow. After melting, the cryostat was filled with liquid nitrogen while the sample temperature was held above the melting point. After the surroundings of the vessel were cooled, a heat exchange gas was admitted. The maximum cooling rate obtained was 4 K·min^{-1}.

Results and Discussion

The experimental molar heat capacities of the measurements on the β-form are given in Table 1. The accuracy of the heat capacity measurements is approximately 0.2%; the precision is generally a factor 10 better. The extreme high values of C_p in the melting region are limited in precision as the temperature increase is very small. The precision of the enthalpy increments, however, is not influenced by the small changes in temperature.

In these measurements no traces of the α-form or of an exothermic effect were found. This makes it reasonably certain that the stable β-form was indeed measured. The enthalpy of melting of the β-form was measured twice. First, the compound as received was measured between 298 K and 350 K. The compound was received as a finely divided powder, probably crystallized from solution. The melting point calculated by extrapolating the plot of the

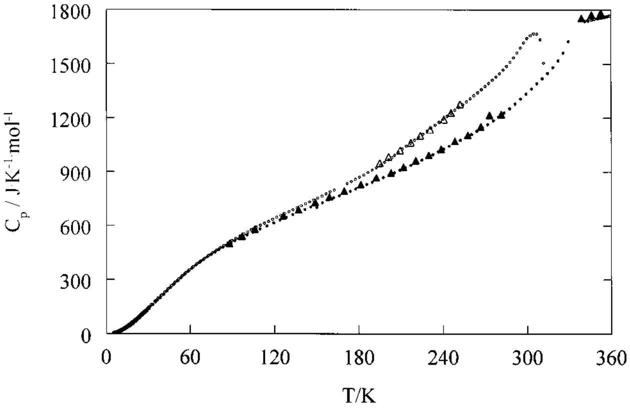

Figure 2. Molar heat capacities of the two crystal forms; closed circles (●) represent the β-form, open circles (○) the α-form; the data of Charbonnet and Singleton (1947) are given by closed (▲) and open triangles (△).

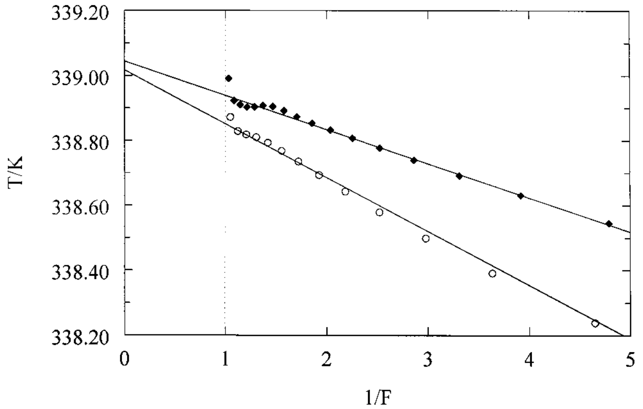

Figure 3. Plot of the reciprocal of the melted fraction (◆) against the equilibrium temperature in the melt. The second melting experiment (o) was used to calculate the purity. The linear function calculated for the second experiment is $T = (339.01 \pm 0.01) - (0.164 \pm 0.003)\cdot(1/F)$. The mole fraction x of the impurity calculated from the slope is 0.0303.

equilibrium temperature versus the reciprocal of the melted fraction to zero was 339.04 K. For the calculation of the baseline all liquid heat capacity data were combined. A linear function was then fitted to the combined data. The linear function is

$$C_p = \{1100.15 + 1.866T/K\}\ J\cdot K^{-1}\cdot mol^{-1} \qquad (1)$$

The standard deviation of the fit, based on 22 datapoints between 340 K and 355 K, is 0.89 J·K^{-1}·mol^{-1}, this corresponds to 0.05% of the mean value of the molar heat capacity in the temperature region. From subsequent measurements it became clear that premelting effects were taking place starting at 220 K (see Figure 2). The melting enthalpy was calculated using a linear fit for the heat capacity of the solid phase from 180 K to 220 K and is given by

$$C_p = \{223.18 + 3.274T/K\}\ J\cdot K^{-1}\cdot mol^{-1} \qquad (2)$$

The standard deviation of this fit, based on 10 datapoints, is 0.73 J·K^{-1}·mol^{-1}, this corresponds to 0.08% of the mean value of the molar heat capacity in this temperature interval. A baseline was constructed based on the solid and the melted fraction in an iterative process. Because the first measurement was started at 298 K, we combined the low-temperature heat capacity data of the β-form with this measurement. This resulted in an enthalpy of melting of 178.1 kJ·mol^{-1}. The heat capacity curves of these series connected very well. This indicates that the product as received was in the β-form. The second melting experiment, performed on a previously melted sample, gave an almost equal melting point of 339.01 K, but a lower value for the enthalpy of melting of 177.2 kJ·mol^{-1}. In Figure 3 the temperatures measured during the melting process are plotted against the reciprocal of the melted fraction. Assuming that the impurity is soluble in the liquid phase, but not in the solid phase, results in a calculated purity of 96.9%, which is much lower than the value given by the supplier. This method of calculating the purity of a compound is based on the presumption that the impurity is soluble in the liquid state, but insoluble in the solid state. The solidification process leaves the impurity in the remaining liquid, and in the following fractional melting process, the impurity is at any moment completely dissolved in the liquid. In the first melting process, however, a solid formed from crystallization out of solution was measured. The rate of diffusion in the solid state is too low to allow the system to come to the equilibrium dictated by the phase diagram with all impurity in the liquid fraction. In Figure 3 the measured equilibrium temperatures are plotted against the reciprocal of the melted fraction for both melting experiments. Completely different curves were found, but extrapolation of the curves to a value $1/F = 0$ gave the same melting point for the pure compound. This emphasizes the necessity to perform purity measurements on a previously melted compound.

The experimental molar heat capacity data of the α-form were measured after cooling the liquid as rapidly as possible. The maximum cooling rate obtainable with the calorimeter was 4 K·min^{-1}. With no reheating performed, the sample was cooled directly to 5 K, and measurements were made from this temperature upward. The experimental data are given in Table 2. The recrystallization process causes the negative heat capacities between 315 and 326 K. These heat capacities are not thermodynamic equilibrium properties. In Tables 3 and 4 the derived thermodynamic properties of the α- and the β-forms are given at integral temperatures. A small exothermic effect was found at a temperature near 168 K. At about 306 K the recrystallization started, resulting in a transformation to the β-form. During this recrystallization process the adiabatic shields were in normal regulation. This implies that the enthalpy path followed by the product and the container could be measured by assuming that the heat exchange with the surroundings was governed by the setting of the shields. This heat exchange was known from empty vessel experiments. Assuming that the enthalpy curve of the liquid can be extrapolated to 318 K gives us the opportunity to calculate the enthalpy of melting of the α-form. The enthalpy values of the measurements of the β-form and the α-form were matched in the liquid phase by adding a value of 29.28 kJ·mol^{-1} to the α-enthalpy values. This value corresponds to the enthalpy difference in these crystal forms at 0 K. Using the fitted heat capacity data of the liquid mentioned above, a value of 108.4 kJ·mol^{-1} was calculated for the enthalpy of melting of the α-form. This corresponds to an entropy of fusion of 340.8 J·K^{-1}·mol^{-1}. In Figure 2 the heat capacity data of both crystal forms are given. The only literature data we found are those of Charbonnet and Singleton (1947), which are also given in this figure. The agreement in the solid state is very good but their heat capacity data in the liquid phase are about 2% higher. In Figure 4 part of the entropy curves for both

Table 2. Experimental Heat Capacity Data and Enthalpy Values of α-Tripalmitin

T (K)	C_p (J·K^{-1}·mol^{-1})	ΔH (J·mol^{-1})	T (K)	C_p (J·K^{-1}·mol^{-1})	ΔH (J·mol^{-1})	T (K)	C_p (J·K^{-1}·mol^{-1})	ΔH (J·mol^{-1})
4.99	4.09	0	104.73	580.97	30485	261.91	1328.4	173647
5.56	4.64	2.49	106.90	590.43	31769	264.57	1345.5	177211
5.83	4.95	3.71	109.82	601.95	33507	267.22	1362.9	180794
6.59	6.56	8	112.71	613.08	35266	269.85	1379.7	184395
7.18	8.23	13.55	115.61	623.95	37055	272.45	1397.4	188016
7.94	10.27	20.58	118.51	634.75	38881	275.04	1415.4	191656
8.70	13.17	29.16	121.41	645.82	40741	277.61	1432.9	195318
9.62	16.85	42.96	124.32	656.79	42633	280.17	1452.0	199000
10.19	19.58	53.97	127.23	667.43	44561	282.70	1472.7	202705
11.32	23.83	77.72	130.14	677.77	46522	285.21	1493.1	206433
11.96	27.08	95.56	133.06	688.66	48516	287.71	1515.4	210183
13.19	32.93	131.33	135.99	699.36	50547	290.18	1540.2	213958
13.87	36.68	156.55	138.92	709.97	52609	292.63	1567.4	217761
15.21	43.77	208.97	141.84	721.12	54703	295.05	1595.2	221595
15.91	47.66	242.78	144.77	732.23	56833	297.45	1623.9	225459
17.36	56.16	316.68	147.71	742.88	58995	299.83	1647.6	229350
18.08	60.75	360.87	150.64	753.98	61194	302.19	1664.3	233261
19.63	70.10	460.12	153.58	765.25	63427	304.54	1673.9	237186
20.37	75.04	516.26	156.53	777.18	65696	306.89	1671.7	241113
21.96	85.93	642.76	159.47	788.97	68000	309.25	1640.7	245021
22.73	91.53	713.12	162.41	797.44	70338	311.67	1511.3	248834
24.38	103.42	871.74	165.39	771.62	72674	315.67	−122.5	250366
25.16	109.52	958.17	168.42	755.15	74984	326.40	−994.4	242125
26.87	121.55	1153	171.45	833.77	77388	334.98	2183.1	235509
27.70	126.28	1258	174.42	845.76	79889	336.00	4344	238635
29.49	139.02	1495	177.38	857.78	82403	336.76	9166	243595
30.36	145.29	1620	180.33	870.18	84952	337.31	16732	250127
32.01	158.80	1871	183.28	882.90	87542	337.64	26301	256969
34.54	178.89	2293	186.23	896.19	90165	337.87	37452	263970
36.84	195.46	2723	189.18	909.55	92830	338.03	49807	271059
39.17	210.89	3198	192.13	923.14	95535	338.16	63348	278201
41.57	228.58	3726	195.08	937.49	98278	338.26	78177	285382
44.01	246.97	4305	198.03	952.00	101063	338.35	94133	292588
46.47	264.91	4934	200.98	967.19	103892	338.42	112178	299814
48.96	282.70	5618	203.41	976.71	106261	338.48	132985	307057
51.50	300.66	6357	205.31	987.81	108125	338.53	155098	314314
54.06	318.11	7152	207.74	1004.37	110550	338.57	179485	321582
56.66	335.89	8001	210.69	1022.21	113538	338.61	208771	328859
59.29	352.45	8906	213.64	1039.27	116572	338.64	240618	336144
61.94	369.04	9862	216.58	1056.56	119658	338.67	281298	343435
64.62	385.21	10871	219.53	1073.81	122798	338.69	336073	350732
67.32	400.85	11934	222.47	1090.98	125987	338.71	422703	358035
70.04	416.31	13047	225.42	1108.28	129227	338.73	602362	365344
72.79	431.47	14210	228.36	1125.63	132507	338.74	784786	372657
75.55	446.33	15422	231.27	1142.53	135814	338.75	881726	379975
78.32	460.68	16680	234.17	1160.61	139145	338.76	364177	387285
81.11	474.80	17986	237.04	1177.49	142502	338.79	162166	394570
83.92	488.71	19338	239.88	1194.79	145878	339.46	4250	400931
86.74	502.10	20735	242.71	1211.71	149277	341.24	1737.6	405649
89.57	515.34	22176	245.51	1228.54	152697	343.53	1741.4	409629
92.42	528.08	23659	248.29	1245.74	156138	345.82	1745.0	413616
95.27	540.69	25184	251.05	1262.94	159598	348.10	1749.3	417602
98.13	552.94	26748	253.79	1277.67	163078	350.38	1754.5	421594
101.00	563.68	28350	256.52	1293.25	166579	352.66	1757.6	425594
103.30	575.42	29661	259.22	1310.93	170102	354.93	1761.9	429595

forms are given, the entropy of the α-form could not be measured above 300 K because the recrystallization is not a reversible process. The entropy values of the α-form above 300 K were obtained by extrapolation. The curves were calculated assuming that both crystal forms have zero entropy at 0 K. If this assumption is correct and the entropy of fusion of the α-form (calculated from the enthalpy of fusion divided by 318 K) is used, then the calculated entropy of the liquid formed from the α-form should coincide with the extrapolated entropy of the liquid formed from the β-form. An alternate statement is that the relative Gibbs energy curves of the α-form and the back-extrapolated liquid should cross at 318 K. This is not the case, however, because the curves cross at 305 K. Several explanations for this discrepancy can be considered.

This discrepancy is due to the experimental error in the determination of the enthalpy of fusion of the α-form. The exothermic effect during the recrystallization leads to a relatively rapid increase in temperature of the vessel. During this effect the shield regulation system does follow this temperature increase. Thus we estimate that in the worst-case scenario an error of 100 μW in the heat exchange with the surroundings could be made. This would lead to an error in the enthalpy increment between the metastable solid and the liquid state of 600 J·mol^{-1}. This error is small compared to the difference in Gibbs energy at 318 K, which is about 5400 J·mol^{-1}.

It is possible that during the fast cooling process not only the α-form was crystallized, but that some of the solid transformed to the β-form. If this were the case, the calculated melting point of the α-form would be higher than 318 K, as the mixture formed is closer to the stable β-form.

The cooling of the α-form can lead to the arrest of certain realization states, comparable to a glass transition. This

Table 3. Thermodynamic Properties at Selected Temperatures for α-Tripalmitin[a]

T (K)	C_p (J·mol^{-1}·K^{-1})	$S°$ (J·mol^{-1}·K^{-1})	$H°(T) - H°(0)$ (J·mol^{-1})	Φ_m^0 (J·mol^{-1}·K^{-1})
10	18.66	6.220	29332	−2926.9
15	42.63	18.04	29481	−1947.3
20	72.56	34.30	29768	−1454.0
25	108.26	54.24	30218	−1154.4
30	142.68	77.02	30845	−951.1
35	182.38	102.01	31658	−802.5
40	216.90	128.63	32657	−687.7
45	254.27	156.34	33835	−595.5
50	290.08	184.99	35196	−518.9
55	324.57	214.27	36733	−453.6
60	356.91	243.92	38438	−396.7
65	387.46	273.71	40300	−346.2
70	416.07	303.48	42309	−300.9
75	443.43	333.13	44459	−259.6
80	469.19	362.57	46741	−221.6
85	493.88	391.77	49149	−186.4
90	517.29	420.66	51677	−153.5
95	539.50	449.23	54320	−122.55
100	559.88	477.44	57070	−93.26
105	582.15	505.30	59926	−65.42
110	602.65	532.87	62889	−38.85
120	640.43	586.93	69105	11.05
130	677.24	639.67	75697	57.39
140	714.07	691.21	82653	100.83
150	751.54	741.76	89982	141.88
160	791.14	791.51	97693	180.93
170	794.97	838.73	105481	218.26
180	868.79	887.08	113942	254.07
190	913.27	935.23	122850	288.66
200	962.16	983.30	132222	322.19
210	1018	1031	142101	354.81
220	1077	1080	152574	386.68
230	1135	1129	163633	417.90
240	1195	1179	175286	448.57
250	1256	1229	187542	478.78
260	1316	1279	200395	508.61
270	1381	1330	213878	538.09
280	1451	1382	228029	567.30
290	1538	1434	242954	596.28
298.15	1632	1478	255867	619.78
300	1649	1488	258902	625.10
310	1615	1536	273600	653.42
318[b]	1667	1578	286753	676.26
318[c]	1693.5	1936	395113	693.5

[a] M = 807.32 g·mol^{-1}; $\Phi_m^0 \overset{def}{=} \Delta_0{}^T\Delta S_m^0 - \Delta_0{}^T H_m{}^0/T$. [b] Solid extrapolated. [c] Liquid back-extrapolated.

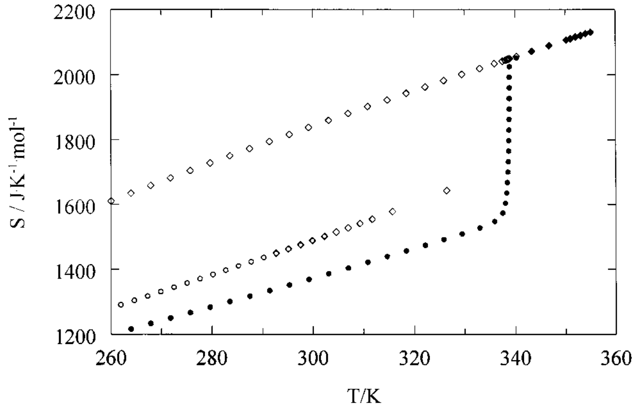

Figure 4. The entropies of the α-form (○) up to 300 K and of the β-form (●) up to the liquid; the back-extrapolated liquid entropy (◇).

would lead to a zero entropy for the α-form. A zero entropy of about (18 ± 2) J·K^{-1}·mol^{-1} results in the coincidence of the calculated and the experimentally observed (by DSC) melting point. This zero entropy corresponds to 8 to 9 realization states. It is tempting to attribute these states (2^3 or 3^2) to the arrangement of the fatty acid chains. If each chain is frozen randomly into one of two possible states this would lead to a zero entropy of R·ln(2^3), or 17.3 J·K^{-1}·mol^{-1}. X-ray data at low temperature are needed to support this assertion.

Table 4. Thermodynamic Properties at Selected Temperatures for β-Tripalmitin

T (K)	C_p (J·mol^{-1}·K^{-1})	$S°$ (J·mol^{-1}·K^{-1})	$H°(T) - H°(0)$ (J·mol^{-1})	Φ_m^0 (J·mol^{-1}·K^{-1})
10	12.45	4.803	35.50	1.253
20	62.25	26.97	383.69	7.789
30	133.29	65.56	1359	20.25
40	210.88	114.88	3092	37.58
50	286.53	170.16	5583	58.49
60	354.96	228.62	8801	81.95
70	413.84	287.89	12653	107.13
80	464.14	346.53	17050	133.40
90	507.72	403.76	21913	160.28
100	546.22	459.32	27190	187.42
110	582.69	513.12	32838	214.59
120	617.40	565.29	38836	241.66
130	651.43	616.07	45182	268.51
140	684.41	665.55	51861	295.11
150	702.40	713.66	58836	321.42
160	748.81	760.73	66131	347.41
170	779.89	807.04	73772	373.09
180	812.11	852.52	81730	398.46
190	844.45	897.30	90014	423.54
200	877.86	941.46	98625	448.34
210	912.03	985.11	107572	472.86
220	947.86	1028	116870	497.13
230	985.81	1071	126537	521.16
240	1026	1114	136592	544.98
250	1067	1157	147054	568.60
260	1109	1199	157925	592.04
270	1156	1242	169244	615.33
280	1208	1285	181057	638.48
290	1270	1329	193440	661.52
298.15	1327	1365	204022	680.25
300	1340	1373	206489	684.49
310	1401	1414	219499	706.71
320	1486	1461	233914	729.55
330	1632	1508	249389	752.42
339.03[b]	1333	1521	25494	770.78
339.03[c]	1733	2044	431517	770.78
350	1753	2100	450637	811.55
360	1772	2149	468261	848.00

[a] M = 807.32 g·mol^{-1}; $\Phi_m^0 \overset{def}{=} \Delta_0{}^T\Delta S_m^0 - \Delta_0{}^T H_m{}^0/T$. [b] Solid, extrapolated. [c] Liquid, back-extrapolated.

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