Triglyceride Property Calculator 3.3_b.1

User and methods manual / Solid fat content of TAG mixtures

Enter the triacylglycerol (TAG) composition of a fat to calculate the fraction of its mass that is crystalline at each temperature. TPC can also estimate how much of that solid mass is β' or β. The required input is a TAG recipe with the fatty acids identified at the three glycerol positions. A fatty-acid profile alone does not specify that recipe.

Run your first SFC curve

1. Open Mixture SFC. Select the Mixture SFC tab. To run the calculator locally, extract the 3.3_b.1 ZIP and follow "Start the calculator" in the README. Open http://127.0.0.1:5000/ once Flask starts.

2. Paste a recipe or select Load CSV. Enter weight percentages of the fat portion, summing to 100. POS means palmitic, oleic and stearic at sn-1, sn-2 and sn-3, respectively. Paste these four lines to reproduce the example on page 2.

```
notation_version,TAG,wt_percent
3.3,POP,22.71
3.3,POS,22.71
3.3,SOS,54.58
```

3. Choose the model. For this example, select β only and Use fitted Wesdorp parameters where available. Leave β packing on Automatic and tick Compare total SFC with the symmetric model. A new session defaults to β' only and the symmetric TPC 3.2 model.

4. Calculate and export. Use 32 to 43 °C in steps of 0.125 °C, then select Calculate SFC. For a single point, set Start and End to 39 °C. Save recipe CSV preserves the notation. Download results CSV preserves the profile, model choices and interaction coverage.

Entering other TAGs

TPC accepts a TAG column or three columns named sn1, sn2 and sn3. Preserve the order of the chains. Common codes are P (palmitic), S (stearic), O (oleic), M (myristic), L (lauric) and J (linoleic).

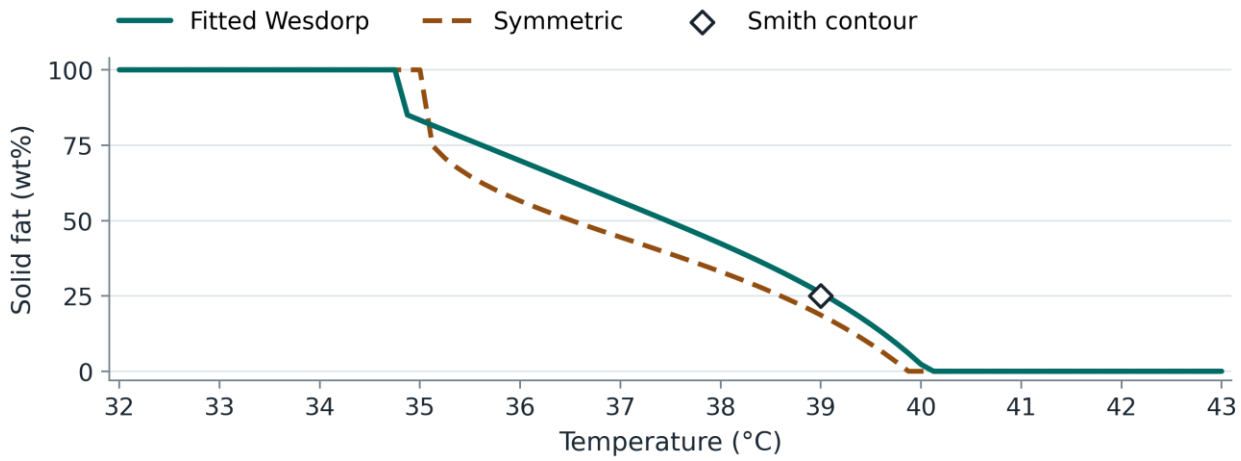
Check older recipes containing E. Recipes for this release still use notation_version=3.3. E = elaidic and Er = erucic. EEE is trielaidin and ErErEr is trierucin. In 3.2, D meant elaidic and E meant erucic. For an unlabelled CSV containing E, select its original notation.

Which result should I report?

For a sample identified as β' by diffraction, choose β' only. If the crystal form is unknown, run β' only and β only to see how much the assumption changes SFC. For the equilibrium prediction when both families are accessible, choose Both forms allowed at equilibrium. Report the temperature, allowed forms, interaction model and number of pairs covered by fitted data.

Reading an SFC–temperature curve

At 39 °C, the same POP/POS/SOS recipe gives 25.99% solid fat with fitted parameters and 18.65% with symmetric parameters.



Both lines are TPC calculations with β allowed. The diamond is one reading from Smith's experimental 25%-solid contour (1988) as reproduced by Wesdorp et al. (2013), Fig. 9.48d. The three fitted pairs all use β-3. The diagram's composition basis is unspecified. This example treats its axes as weight fractions.

What the two plot settings mean

"SFC and crystal mass in the mixture" uses the whole fat as denominator. For example, if 100 g of fat contains 30 g β' and 10 g β, the total SFC is 40 wt%. "β' and β shares of the solid fat" uses only the 40 g of crystals. The same sample is then 75% β' and 25% β within its solids. These shares are undefined when the fat is fully liquid.

Choose β' only or β only to ask what equilibrium looks like within a given crystal family. Both forms allowed at equilibrium lets the calculation determine their proportions at each temperature. A conditioned sample can retain a metastable form, so record the thermal history and compare the predicted proportions with diffraction where possible.

How closely do the curves follow experimental data?

Release benchmark · mean absolute error	Symmetric	Fitted[1]
POP/POS/SOS, SFC at 10 contour points	21.61 points	19.26 points
Same recipes, temperature at 25% SFC	0.44 °C	0.54 °C
Canola oil / fully hydrogenated palm stearin, 7 NMR points	3.69 points	3.69 points

[1] Fitted where available. SFC errors are percentage points. The ten ternary readings share one steep melting region and the fitted binaries and contour come from the same experimental source. In the 30:70 spread, only 5 of 4,465 pairs had β'-2 fits. Pair coverage helps explain why the two spread curves nearly coincide.

Which melting properties does TPC use?

Single TAG and Batch show the measurements and both Seilert fits. Mixture SFC selects one melting temperature and one fusion enthalpy per TAG for each allowed crystal form.

Reading the Single TAG and Batch results

The public reports give experimental values alongside Seilert Fit I and Fit II. A note identifies a fit that predicts β melting below β' or gives a nonpositive fusion enthalpy. Batch saves these notes in the Model_warnings column. The historical Wesdorp–Moorthy and group-contribution values are available through a research export (see below).

POS as a worked example

Mixture SFC selects each property independently, using the experimental lookup first and Fit I for a missing value. For POS, the lookup supplies all four inputs.

Experimental input for POS	β'	β
Melting temperature (°C)	31.6	37.1
Fusion enthalpy (kJ/mol)	119.2	150

Arishima et al. measured 31.6 °C and 119.2 kJ/mol for pseudo-β' rac-POS. The separate 31.0 °C observation in Wesdorp's thesis was originally labelled β' and excluded from the fit (frequency zero). The 2013 book dropped the prime on that row. The Single TAG tab links to the experimental sources and the historical POS observations.

Why the two SFC tabs can give different results

Legacy SFC takes its melting temperatures and enthalpies from historical Model A, even where measurements exist. It sums a separate melting curve for each TAG by mass. For POS, Model A predicts 40.8 °C for β' and 36.2 °C for β. A recipe using either form displays an order warning beside the download and on the Warnings sheet of the Excel workbook.

On the Single TAG page, Seilert Fit I also reverses the order for POS (β' 37.4 °C and β 36.6 °C). Fit II gives β' 35.8 °C and β 37.0 °C. The equilibrium curve uses the experimental POS values in the table.

Seilert melting predictions retain the workbook's empirical counting rule for unsaturated chains. For triolein (OOO), that rule gives a nonzero oleic–linoleic term even though triolein contains no linoleic acid. Fusion enthalpy uses a separate equation with single-chain counts.

Research access. Send report_columns=research to POST /compute or POST /upload_batch to include the historical predictions and their order warnings.

From a recipe to phase amounts

At each temperature the solver redistributes every TAG among the allowed phases. The distribution with the lowest total Gibbs energy determines the predicted mass of crystals.

1 Pure TAGs set the melting scale

For each TAG and permitted crystal family, TPC selects its melting temperature and fusion enthalpy independently. It uses an experimental lookup value where available and fills a missing value with the Seilert PI,L prediction. The input table records the source of each number. A missing usable value from both sources prevents the calculation.

Use each pure liquid as its own zero of Gibbs energy. The pure solid's energy relative to that liquid is the melting term below. T and T_m are in kelvin, ΔHfus in J/mol and R is the gas constant. TPC neglects the solid–liquid heat-capacity difference.

$$b_i^p(T) = \frac{g_i^{p,0} - g_i^{L,0}}{RT} = \frac{\Delta H_{\mathrm{fus},i}^p}{R}\left(\frac{1}{T_{m,i}^p} - \frac{1}{T}\right)$$

Below its melting point this term is negative, so the pure solid is favoured. At its melting point the pure liquid and solid have equal Gibbs energies.

2 Each candidate phase has a molar Gibbs energy

$$\frac{g^p}{RT} = \sum_i x_i^p\, b_i^p + \sum_i x_i^p \ln x_i^p + \frac{g^{E,p}}{RT}$$

The terms represent the pure-component energies, ideal entropy of mixing, and excess energy from interactions. All mole fractions are local to phase p. The liquid is ideal in TPC, with b = 0 and $g^E = 0$. Its entropy of mixing still contributes to the equilibrium.

3 Minimize total energy while conserving each TAG

$$\min_{\{n_i^p\}} \quad \frac{G}{RT} = \sum_p N_p \frac{g^p}{RT}, \qquad \sum_p n_i^p = n_i^0, \qquad n_i^p \geq 0$$

For a 100 g recipe, divide each TAG mass by its molar mass M_i to get its starting moles n_i^0. The variables n_i^p are the moles assigned to each phase. Their sum within p gives N_p, and $x_i^p = n_i^p/N_p$ for a phase that is present. Distinct solid compositions can coexist within one family. The multicomponent solver uses multiple starting points and stability checks. A global minimum is sought but cannot be certified for every recipe.

4 Convert the equilibrium solids back to mass

$$\mathrm{SFC}\ (\mathrm{wt\%}) = 100\ \frac{\sum_{p\,\in\,\mathrm{solids}} \sum_i n_i^p\, M_i}{\sum_i n_i^0\, M_i}$$

Restrict the numerator to β' or β to obtain the mass percentage of the whole fat in that crystal family.

How TPC assigns Margules parameters

TPC uses either a chain-length estimate or a fit to an experimental phase diagram for each pair in a crystal.

From chain lengths to a symmetric Margules parameter

To calculate the isomorphism index ε_{ij} for TAGs i and j, compare their carbon counts C_{ik} and C_{jk} at each sn position k. The numerator sums the unmatched carbons across all three positions. The denominator sums the overlap, taking the smaller count at each position.

$$\varepsilon_{ij} = 1 - \frac{\sum_{k=1}^{3} |C_{ik} - C_{jk}|}{\sum_{k=1}^{3} \min\left(C_{ik}, C_{jk}\right)}$$

Wesdorp's empirical equations give one dimensionless parameter for both directions, $h_{ij} = h_{ji} = A_{ij}/(RT)$. The choice of equation depends on the crystal family.

β' crystals	β crystals
$h_{ij}^{\beta'} = 18.2 - 19.5\,\varepsilon_{ij}, \quad \varepsilon_{ij} \le 0.93$ h = 0 when $\varepsilon_{ij} > 0.93$	$h_{ij}^{\beta} = 35.9 - 35.8\,\varepsilon_{ij}, \quad \varepsilon_{ij} \le 0.98$ h = 0 when $\varepsilon_{ij} > 0.98$

Worked example for SOS and POP

SOS has (18, 18, 18) carbons and POP has (16, 18, 16). The unmatched total is 2 + 0 + 2 = 4 and the overlap is 16 + 18 + 16 = 50. Thus ε = 1 − 4/50 = 0.92. For β', h = 18.2 − 19.5 × 0.92 = 0.260. For β, h = 35.9 − 35.8 × 0.92 = 2.964.

SSS and OOO illustrate a limitation. Both have (18, 18, 18), so ε = 1 and h = 0 in both families. A carbon-count index cannot capture the packing effect of oleic acid's cis double bond.

Where the coefficients enter the solid free energy

For a crystal of composition x, h_{ij} equals ln γ_i for TAG i at infinite dilution in host j. A positive value penalizes incorporation relative to ideal mixing. A negative value favours it. Each pair contributes once to the excess molar Gibbs energy of phase p.

$$\frac{g^{E,p}}{RT} = \sum_{i<j} x_i\, x_j\, \frac{h_{ij} x_j + h_{ji} x_i}{x_i + x_j}$$

For a symmetric pair the contribution simplifies to $h_{ij}x_i x_j$. In fitted mode, the β-3 values for SOS–POP are 5.0 for SOS dilute in POP and 1.5 for POP dilute in SOS. Uncovered pairs retain the symmetric estimate.

Automatic selects one packing per family. Conflicting evidence gives symmetric estimates unless a packing is specified. Pure melting properties are family-level. TPC holds fitted A/RT constant over temperature. Wesdorp held A constant. Converting the fits would require their individual reference temperatures.

Fitted Margules parameters in TPC 3.3_b.1

All 19 enabled TAG-pair and packing combinations. Read h_{12} as TAG 1 dilute in a TAG 2 crystal. Read h_{21} as TAG 2 dilute in a TAG 1 crystal.

Packing	TAG 1	TAG 2	$h_{12} = A_{12}/RT$	$h_{21} = A_{21}/RT$	Ch. 9 table
β-2	SSS	SES	0 ± 0.5	0.8 ± 0.5	9.36
β-2	SSS	SSE	0.1 ± 0.5	0.7 ± 0.5	9.36
β-2	SSS	SEE	0 ± 1	0 ± 1	9.36
β-2	SSS	EEE	0 ± 0.2	0 ± 0.2	9.36
β-2	SES	SSE	0 ± 0.5	0 ± 0.5	9.36
β-2	SSS	PSS	1.1 ± 0.5	2.3 ± 0.5	9.36
β-2	PSS	PPS	1.4 ± 0.5	1.8 ± 0.5	9.36
β-2	PPS	PPP	1.6 ± 0.5	2.3 ± 0.5	9.36
β-2	PSS	SPS	1.4 ± 0.5	2.6 ± 0.5	9.36
β-2	PSS	PPP	2.8 ± 0.5	2.1 ± 0.5	9.36
β-2	SSS	PPP	5.8 ± 1	1.4 ± 1	9.36
β-3	SOS	POS	1.5 ± 0.5	1.1 ± 0.5	9.36
β-3	POS	POP	2.2 ± 0.5	1.0 ± 0.5	9.36
β-3	SOS	POP	5 ± 1	1.5 ± 1	9.36
β'-2	PSP	POP	−3 ± 1	0 ± 0.5	9.33
β'-2	PSP	SSO	−2 ± 1	0 ± 0.5	9.33
β'-2	MPM	POP	0.8 ± 0.4	0.8 ± 0.2	9.35
β'-2	MPM	PPO	0.8 ± 0.5	0.8 ± 0.3	9.35
β'-2	MPM	SSO	2 ± 0.7	2 ± 0.2	9.35

Coefficients are dimensionless. The ± margins are transcribed as published. TPC uses the central values and does not propagate those margins into an SFC uncertainty band. Six fits have equal central values. No β'-3 entry qualifies in this release.

Tracing a value

In Mixture SFC, open Interaction coverage → Fitted pairs and catalogue records. Each entry identifies its two source records. The release includes the 315-record curated catalogue, eligible_pairs.csv and the selection rationale under app/data/wesdorp/.

Primary sources

Wesdorp, L. H. (1990). Liquid–multiple solid phase equilibria in fats. Doctoral thesis, TU Delft. Thesis

Wesdorp et al. (2013). “Liquid–Multiple Solid Phase Equilibria in Fats.” Ch. 9, Structure and Properties of Fat Crystal Networks, 2nd ed. Fig. 9.48d. Chapter

Teles dos Santos, Gerbaud & Le Roux (2013). Chemical Engineering Science 87, 14–22. Article

Karabulut, Turan & Ergin (2004). European Food Research and Technology 218, 224–229. Fig. 1, physical blend. Article

Seilert et al. (2021). “Revisiting a model to predict pure triglyceride thermodynamic properties: parameter optimization and performance.” JAOCS. Article

Arishima, Sagi, Mori & Sato (1991). “Polymorphism of POS. I. Occurrence and polymorphic transformation.” JAOCS 68, 710–715. Table 2. Article