Predefined internal function variables

Defintion	Description	Defintion	Description	Defintion	Description
n_1	number of carbon atoms in FA_1	$P = \min(n_1,n_3)$	shortest outer chain length	n_{lc}	number of linolenic chains
n_2	number of carbon atoms in FA_2	$Q = n_2$	middle chain length	n_{OO}	number of oleic-oleic pairs
n_3	number of carbon atoms in FA_3	$R = \max(n_1,n_3)$	longest outer chain length	n_{EE}	number of elaidic-elaidic pairs
$n = \sum n_i$	total carbon number	$x = Q - P$	chain length difference	n_{ll}	number of linoleic-linoleic pairs
u_1	number of double bonds in FA_1	$y = R - P$	chain length difference	n_{lele}	number of linolenic-linolenic pairs
u_2	number of double bonds in FA_2	n_O	number of oleic chains	n_{Ol}	number of oleic-linoleic pairs
u_3	number of double bonds in FA_3	n_E	number of elaidic chains	n_{Ole}	number of oleic-linolenic pairs
$u = \sum u_i$	total number of double bonds	n_l	number of linoleic chains	n_{lle}	number of linoleic-linolenic pairs

Saturated triglycerides

Predicting the enthalpy and entropy of fusion

$$\Delta H^{sat} = h\,n + h_0 + h_{xy}\,f_{xy} + h_{odd}\,f_{odd}\,f_\beta \quad [1]$$

$$\Delta S^{sat} = s\,n + s_0 + s_{xy}\,f_{xy} + s_{odd}\,f_{odd}\,f_\beta + R\ln 2\,f_{asym}\,f_\beta \quad [2]$$

$$f_{xy} = 2 - \exp\left(-\left(\frac{x - x_0}{k}\right)^2\right) - \exp\left(-\left(\frac{y}{k}\right)^2\right) \quad [3]$$

$$f_{odd} = \begin{cases} 1, \text{if } n_1 \text{ or } n_2 \text{ or } n_3 \text{ is odd numbered} \\ 0, \text{if } n_1 \text{ or } n_2 \text{ or } n_3 \text{ is even numbered} \end{cases} \quad [4]$$

$$f_{asym} = \begin{cases} 1, \text{if } y \neq 0 \\ 0 \text{ if } y = 0 \end{cases} \quad [5]$$

$$f_\beta = \begin{cases} 1, \text{if TAG is in } \beta \text{ polymorph} \\ 0, \text{if TAG is not in } \beta \text{ polymorph} \end{cases} \quad [6]$$

Parameter	Description
h, s	hydrocarbon chain contribution
h_0, s_0	end group contribution
h_{xy}, s_{xy}	contribution of differences in chain length
k, x_0	constant
h_{odd}, s_{odd}	odd chain contribution
A_0, B_0	end group contribution
A_{odd}, B_{odd}	odd chain contribution
A_x, A_{x^2}, A_{xy}, A_y, A_{y^2}, B_x, B_{x^2}, B_{xy}, B_y, B_{y^2}	fitting parameter

$$T_m^{sat} = \frac{\Delta H^{sat}}{\Delta S^{sat}} = \frac{h\,n + h_0'}{s\,n + s_0'} \quad [7]$$

$$h_0' = h_0 + h_{xy}\,f_{xy} + h_{odd}\,f_{odd}\,f_\beta \quad [8]$$

$$s_0' = s_0 + s_{xy}\,f_{xy} + s_{odd}\,f_{odd}\,f_\beta + R\ln 2\,f_{asym}\,f_\beta \quad [9]$$

Re-writing eq. [7] as Taylor series expansion around $\left(\frac{1}{n}\right)$:

$$T_m^{sat} = \frac{h}{s}\left(1 + \left(\frac{h_0'}{h} - \frac{s_0'}{s}\right)\frac{1}{n} - \frac{s_0'}{s}\left(\frac{h_0'}{h} - \frac{s_0'}{s}\right)\frac{1}{n^2} + \cdots\right) \quad [10]$$

Truncating the series and substituting for convenience results in eq. [11]

Predicting the melting point

$$T_m^{sat} = T_{inf}\left(1 + \frac{A^{sat}}{n} - \frac{A^{sat}\,B^{sat}}{n^2}\right) \quad [11]$$

1st approach

$$A^{sat} = A_0 + A_{odd}f_{odd} + A_x x + A_{x^2}x^2 + A_{xy}xy + A_y y + A_{y^2}y^2 \quad [12]$$

$$B^{sat} = B_0 + B_{odd}f_{odd} + B_x x + B_{x^2}x^2 + B_{xy}xy + B_y y + B_{y^2}y^2 \quad [13]$$

2nd approach

$$A^{sat} = \frac{\widehat{h_0}}{h} - \frac{\widehat{s_0}}{s} \quad [14] \qquad B^{sat} = \frac{\widehat{s_0}}{s} \quad [15]$$

$$\widehat{h_0} = h_0 + h_{xy}\,f_{xy} + h_{odd}\,f_{odd}\,f_\beta \quad [16]$$

$$\widehat{s_0} = s_0 + s_{xy}\,f_{xy} + s_{odd}\,f_{odd}\,f_\beta + R\ln 2\;f_\beta\,f_{asym} \quad [17]$$

Unsaturated triglycerides

Predicting the enthalpy of fusion

$$\Delta H^{unsat} = H^{sat} + h_O\,n_O + h_E\,n_E + h_l\,n_l \quad [18]$$

Predicting the melting point

$$A^{unsat} = A^{sat} + A_O\,n_O + A_E\,n_E + A_l\,n_l + A_{le}\,n_{le} + A_{OO}\,n_{OO} + A_{EE}\,n_{EE} + A_{ll}\,n_{ll} + A_{Ol}\,n_{Ol} + A_{Ole}\,n_{Ole} + A_{lle}\,n_{lle} \quad [19]$$

$$B^{unsat} = B^{sat} + B_O\,n_O + B_l\,n_l + B_{le}\,n_{le} \quad [20]$$

Parameter	Description
h_O	oleic chain contribution
h_E	elaidic chain contribution
h_l	linoleic chain contribution
A_O, A_E, A_l, A_{le}, B_O, B_l, B_{le}	correction parameter accounting for oleic, elaidic, linoleic and linolenic acid
A_{OO}, A_{EE}, A_{ll}, A_{lele}	interaction of the same unsaturated FA
A_{Ol}, A_{Ole}, A_{lle}	interaction of different unsaturated FA