1.92: Debye's Heat Capacity Equation Fit to Experimental Data - Another Algorithm

$$n := 30 \qquad i := 1 \ldots n$$

$T_i :=$	$C_i :=$
1	0.000818
3	0.0065
5	0.0243
8	0.0927
10	0.183
15	0.670
20	1.647
25	3.066
30	4.774
35	6.612
40	8.419
45	10.11
50	11.66
55	13.04
60	14.27
65	15.35
70	16.30
80	17.87
90	19.11
100	20.10
120	21.54
140	22.52
160	23.22
180	23.75
200	24.16
220	24.49
240	24.76
260	24.99
280	25.19
300	25.37

The heat capacity data were taken from the *Handbook of Physics and Chemistry* - 72nd Edition, page 5-71. The data are presented in units of Joules/mole/K.

Gas law constant:

$$\mathrm{R} := 8.31451$$

Define Einstein function for heat capacity and first derivative with respect Θ:

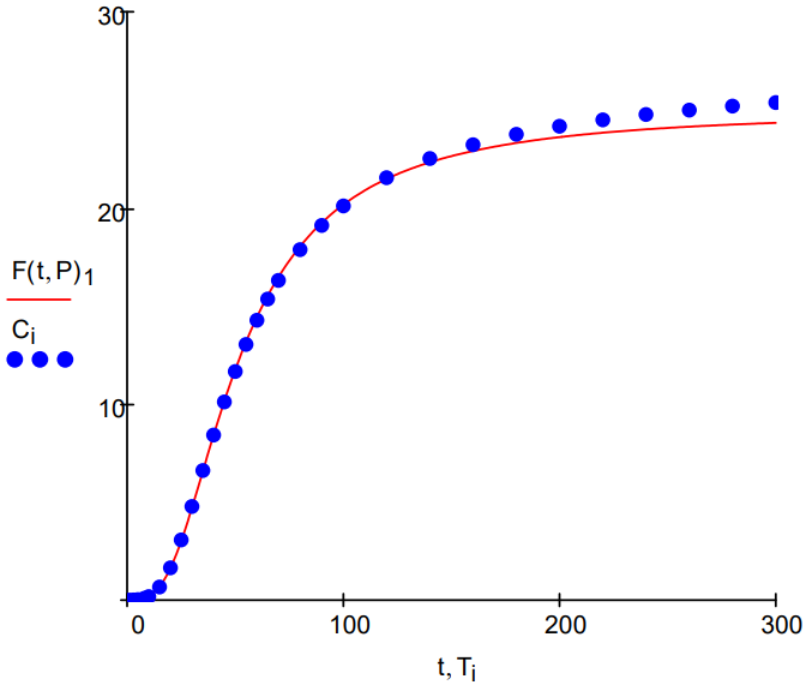
$$F(T,\Theta) = \begin{bmatrix} 9\cdot R\cdot\left(\frac{T}{\Theta}\right)^3\cdot\int_0^{\frac{\Theta}{T}}\frac{x^4\cdot\exp(x)}{(\exp(x)-1)^2}dx \\ \frac{d}{d\Theta}\left[9.R\cdot\left(\frac{T}{\Theta}\right)^3\cdot\int_0^{\frac{\Theta}{T}}\frac{x^4\cdot\exp(x)}{(\exp(x)-1)^2}dx\right] \end{bmatrix}$$

Call genfit to do nonlinear regression analysis.

$$P := \text{genfit}\,(T, C, 200, F) \qquad P = 210.985$$

Plot data and fit:

$$\mathrm{t} := 1\ldots 300$$



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