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Addendum

Addendum to "The vaporization enthalpies and vapor pressures of a series of fatty acids methyl esters for C_{18}, C_{21} to C_{23}, C_{25} to C_{29} by correlation gas chromatography" [Thermochim. Acta 424 (2004) 111–121]

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The vapor pressures of the fatty acid methyl esters reported in this article [1] were evaluated from the vapor pressure equations reported previously in an article by van Genderen et al. [2] processed in the form of the regression equation (Eq. (1)) introduced by Clarke and Glew [3]. In this equation, p is the saturation vapor pressure, T the thermodynamic temperature, θ the chosen reference

$$R\ln\left(\frac{p}{p_0}\right) = -\frac{\Delta_1^{\mathrm{g}}G_{\mathrm{m}}(\theta)}{\theta} + \Delta_1^{\mathrm{g}}H_{\mathrm{m}}(\theta)\left[\frac{1}{\theta}-\frac{1}{T}\right] + \Delta_1^{\mathrm{g}}C^{\circ}_{p,\mathrm{m}}\left[\frac{\theta}{T}-1+\ln\left(\frac{\theta}{T}\right)\right] \quad (1)$$

temperature, p_0 the reference pressure; p_0 was chosen by van Genderen et al. as 1 Pa. Molar values for the Gibbs' free energy, the vaporization enthalpy, and the heat capacity difference between the gas and liquid phases, $\Delta_1^{\mathrm{g}}G_{\mathrm{m}}(\theta)$, $\Delta_1^{\mathrm{g}}H_{\mathrm{m}}(\theta)$ and $-\Delta_1^{\mathrm{g}}C^{\circ}_{p,\mathrm{m}}$, respectively, were computed at several temperatures including $T = 298.15$ K and 350 K. Vapor pressures were calculated at $T = 298.15$ K using the parameters reported by van Genderen et al. [2] for $\theta = 350$ K. The parameters and compounds used in calculating the vapor pressures of the title compounds are reported in Table 1. The vapor pressures calculated from these parameters were also expressed in the form of a third order polynomial Eq. (2), used to model the temperature dependence of vapor pressure. The parameters in Eq.

Table 1
Literature parameters for Eq. (1) and the A–D parameters generated for Eq. (2)

	$\Delta G^{\circ}_{\mathrm{m}}$ (J mol^{-1})[a]	$\Delta H^{\circ}_{\mathrm{m}}$ (J mol^{-1})[a]	$\Delta C^{\circ}_{p,\mathrm{m}}$ (JK^{-1} mol^{-1})[a]	$10^{-8}A$[b]	$10^{-6}B$[b]	C[b]	D[b]
Methyl dodecanoate	−11,324	71,421	−113.5	2.18708	−2.72723	1633.21	4.862
Methyl tridecanoate	−8,987	73,955	−91.8	1.76893	−2.20581	−626.33	7.233
Methyl tetradecanoate	−6,534	79,828	−120.7	2.32582	−2.90023	1270.55	5.341
Methyl pentadecanoate	−4,346	82,100	−102.4	1.97319	−2.46051	−651.20	7.312
Methyl hexadecanoate	−1,657	93,363	−213.7	4.11787	−5.13488	8019.92	−1.553
Methyl octadecanoate	3,011	98,021	−157.9	3.04264	−3.79409	2433.18	4.364
Methyl nonadecanoate	4,827	101,170	−159	3.06384	−3.82052	2153.49	4.705
Methyl eicosanoate	7,308	109,200	−203	3.91169	−4.87777	5151.12	1.941

[a] Literature parameters for Eq. (1) at $\theta = 350$ K [1].
[b] Evaluated using the vapor pressures calculated from Eq. (2) using a reference pressure, p_0, of 101,325 Pa.

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Table 2
Vapor pressure parameters (*A*–*D*) evaluated for FAMEs C_{18}, C_{22} to C_{23} and C_{25} to C_{28}

	$10^{-8}A$	$10^{-6}B$	C	D
Methyl heptadecanoate	3.20885	−3.99382	3615.89	3.0564
Methyl heneicosanoate	4.20126	−5.23876	5943.62	1.2615
Methyl docosanoate	4.62998	−5.77717	7293.43	0.0632
Methyl tetracosanoate	5.48008	−6.84544	9971.29	−2.3130
Methyl pentacosanoate	5.98677	−7.47838	11631.82	−3.8127
Methyl hexacosanoate	6.43086	−8.03301	13047.85	−5.0815
Methyl heptacosanoate	6.85197	−8.56341	14379.54	−6.2620
Methyl octacosanoate	7.29147	−9.11763	15787.58	−7.5139

(2) refer to a reference pressure, p_0, of 101,325 Pa, which we neglected to mention in the article. This was also the reference pressure used to calculate the vapor pressures of the unsaturated FAMEs reported recently [4]. We apologize for any confusion this may have caused. The parameters (*A*–*D*) of Eq. (2) for methyl dodecanoate to methyl eicosanoate exclusive of methyl heptadecanoate are included in Table 1 and of methyl heptadecanoate, heneicosanoate, docosanoate, and tetracosanoate through to methyl octacosanoate remain unchanged and are reported in Table 2.

$$\ln\left(\frac{p}{p_0}\right) = AT^{-3} + BT^{-2} + CT^{-1} + D \quad (2)$$

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