JOURNAL OF PHYSICAL CHEMISTRY, 2025, Vol. 99, No. 1, c. 21–28

CHEMICAL THERMODYNAMICS AND THERMOCHEMISTRY

SATURATED VAPOR PRESSURES AND ENTHALPIES OF VAPORIZATION OF MALIC ACID ESTERS

Yu. F. Yamshchikova, S. V. Portnova, and E. L. Krasnykh*

Samara State Technical University, Samara, Russia

**e-mail: kinterm@samgtu.ru*

Received April 16, 2024
Revised April 16, 2024
Accepted May 08, 2024

Abstract. The saturated vapor pressures of complex malic acid diesters and linear C_1–C_5 alcohols are determined using the transpiration method in the temperature range of 303–369 K. The enthalpies of vaporization of esters at 298.2 K are determined on the basis of the obtained data. Correlations of the enthalpies of vaporization on Kovats indices and number of carbon atoms are obtained. The contributions

of the hydroxyl group and intermolecular hydrogen bonds to $\Delta_{vap}H^{\circ}(298.15\ K)$ are estimated. The author's QSPR method for calculating the values of the enthalpies of vaporization of esters of hydroxy acids is modified.

Keywords: *malic acid esters, saturated vapor pressures, enthalpy of vaporization, QSPR method*

DOI:10.31857/S00444537250102e6

Malic acid is a dicarboxylic hydroxy acid that has a wide range of applications. Malic acid is mainly used in the food industry as an acidity regulator and flavoring agent [1–3]. Malic acid based polymers are used in medicine as surgical threads and implants [4–8]. In pharmaceutical chemistry, this acid is used to produce nanosystems for drug delivery [9, 10]. In addition, malic acid and its esters are used as effective green solvents [11, 12].

Malic acid can be produced in petrochemical and enzymatic ways. Conventionally, the acid is produced chemically by hydration of maleic anhydride under high temperature and pressure conditions. As the shift to green chemistry has been increasingly emphasized in recent decades, production by biotechnology based on renewable substrate is preferred [13, 14]. At the same time, the biotechnological process should be economically competitive, which is the most important factor for the commercialization of the process. The US Department of Energy rates malic acid as one of twelve promising precursors that can be produced in large quantities from biomass [15]. Market volume data for malic acid ranges from 60,000 to 200,000 tons per year [13, 16]. With the ever-increasing demand, production is forecasted to increase by another 150,000 tons per year in the coming years [13]. As part of the development of green chemistry, this method will compete with the petrochemical method of maleic anhydride production, which is estimated at 3.2 million tons in 2023 [17].

Currently, the cost of malic acid produced by biotechnological method accounts for more than 50% of the product separation [18]. The application of reaction-distillation processes to obtain malic acid esters will reduce the product cost [19, 20]. Accordingly, for the distillation unit technology to be designed, precision data on saturated vapor pressures and enthalpies of vaporization of ethers are required.

The available published data on malic acid esters is represented only by [21], which gives the coefficients of the Antoine equation for methyl and ethyl ethers.

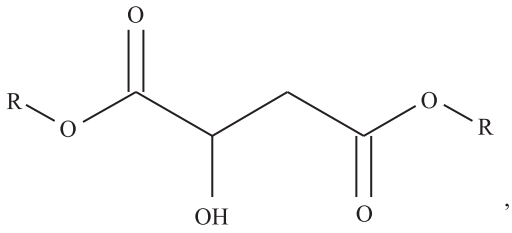
This work continues our studies on determination of thermodynamic and physicochemical properties of esters of natural hydroxy acids [22–24].

EXPERIMENTAL PART

Samples of esters were prepared by esterification of malic acid with the respective alcohol. The synthesis technique is described in [24]. The esters of the following structure were synthesized (Fig. 1).

The purity of the samples was determined by gas-liquid chromatography using a Crystal-2000M chromatograph equipped with a flame ionization detector, a capillary column of 100 m × 0.2 mm × × 0.5μm with grafted fixed liquid phase DB-1. The water content of the esters was determined by GLC with a thermal conductivity detector and a 1 m long nozzle column with Chromosorb HP 10% phase. No water was detected in any of the ester samples. Table 1 shows the purity of the resulting esters.

The saturated vapor pressures of the studied esters were determined by the transfer method, and the



R = CH_3-, CH_3-CH_2-, CH_3- CH_2-CH_2-, CH_3- CH_2- CH_2-CH_2-, CH_3-CH_2- CH_2- CH_2- CH_2-.

Fig. 1. Structure of complex diesters of malic acid.

Table 1. Characteristics of samples of the produced malic acid esters

Ester	CAS RN	Purity of esters (GLC), wt.
Dimethylmalate	1587-15-1	0.999
Diethylmalate	7554-12-3	0.999
Di-n-propylmalate	1587-17-3	0.998
Di-n-butylmalate	1587-18-4	0.998
Di-n-pentylmalate	–	0.997

values of the enthalpies of vaporization of the esters were calculated on the basis of these pressures. The experimental and calculation methods are given in [23, 25, 26].

DISCUSSION OF RESULTS

Saturated Vapor Pressures and Enthalpies of Vaporization

The obtained values of saturated vapor pressures, values of $\Delta_{vap}H^o$ (298.15 K), and values of the change in the heat capacity of the gas-liquid transition ($\Delta_l^g C^o_{p,m}$) are given in Table 2, and Figs. 2 and 3 show the dependences of the logarithms of saturated vapor pressures (obtained in this work and publication [21]) on the inverse temperature for dimethyl- and diethylmalates.

As we can see from Figs. 2 and 3, the saturated vapor pressures of dimethyl- and diethylmalates obtained by us are slightly lower than the published values. This may be due to the fact that work [21] only gives data on the coefficients of the Antoine equation and lacks data on the purity of the samples and the method of determining the pressures. At the same time, the values $\Delta_{vap}H^o$ (298.15 K) calculated from the values of saturated vapor pressures, given the error, are comparable to each other (74.4 ± 1.3 kJ mol^{-1} and 75.1 kJ mol^{-1} for dimethylmalate, 76.4 ± 1.1 kJ mol^{-1} and 78.1 kJ mol^{-1} for diethylmalate).

To check the internal consistency of the experimental results for $\Delta_{vap}H^o$ (298.15 K), we correlated the values $\Delta_{vap}H^o$ (298.15 K) with the number of carbon atoms in the alcohol moiety and with the Kovats indices [22, 23, 28] (Fig. 4). As we can see from the graph, the value $\Delta_{vap}H^o$ (298.15 K) of dimethylmalate falls out of the linear dependence. The same behavior is characteristic of dimethylsuccinate (Fig. 4) [29, 30]. This fact may be due to the differences of inter- and intramolecular hydrogen bonds in liquid and gas phases, entropic factor [22, 23], and high dipole moment of aliphatic ethers [31].

In general, the correlation of the values $\Delta_{vap}H^o$ (298.15 K) on the number of carbon atoms of the alcohol moiety (n_C) at $n_C \geqslant 2$ is described by the equation

$$\Delta_{vap}H^o\left(298.15\ K\right) = \\ = \left(7.24 \pm 0.43\right) \times n_C + \left(61.21 \pm 1.57\right), \quad (1)$$
$$R^2 = 0.993.$$

The correlation of the values $\Delta_{vap}H^o$ (298.15 K) on the Kovats indices (J_x) on the nonpolar DB-1 phase and at T = 503.15 K [24] is described by the equation

$$\Delta_{vap}H^o\left(298.15\ \text{K}\right) = \\ = \left(0.0381 \pm 0.002\right) \times J_x + \left(28.42 \pm 3.50\right), \quad (2)$$
$$R^2 = 0.993.$$

The regression coefficients (R^2) in Eqs. (1) and (2) show good agreement of the results. Moreover, these equations can be used to calculate $\Delta_{vap}H^o$ (298.15 K) when $n_C > 5$.

In [22, 23], it was shown that esters of glycolic and lactic acids have intra- and intermolecular hydrogen bonds due to the presence of a hydroxyl group in the ester molecules. It is logical to assume that the same interactions would be characteristic of dialkylmalates. The contribution of the hydroxyl group and intermolecular hydrogen bonds to $\Delta_{vap}H^o$ (298.15 K) of hydroxycarboxylic acid esters was evaluated using the experimental values of the enthalpy of vaporization and the concept of homomorphic compounds [32, 33]. The esters of alkyl acetate, alkyl propionate, and dialkyl succinate esters were used as homomorphic homologs for alkyl glycolates, alkyl lactates, and dialkyl malates, respectively. The values $\Delta_{vap}H^o$ (298.15 K) for homomorphic compounds were taken from the National Institute of Standards and Technology (NIST) ChemistryWebBook thermodynamic research

Table 2. Results of determination of saturated vapor pressures of malic acid esters.

T, K	m, mg	V(He), dm^3	T_a, K	Flow rate, dm^3 h^{-1}	p, Pa	$u(p)$, Pa	$\Delta_l^g H_m^o$, kJ/mol
Dimethylmalate: $\Delta_{vap}H^o\,(298.15\ \mathrm{K}) = (74.4 \pm 1.3)\ (\mathrm{kJ\cdot mol^{-1}})\ \ln p = \frac{388.3}{R} - \frac{114870.1}{RT} - \frac{135.6}{R}\ln\left(\frac{T}{298.15}\right)$							
303.5	1.64	10.714	301.2	10.71	2.36	0.08	73.66
305.5	1.80	9.424	298.2	9.42	2.92	0.10	73.39
307.7	2.66	10.209	298.2	9.42	3.99	0.12	73.09
309.5	2.52	8.434	300.7	7.23	4.61	0.14	72.85
311.6	1.80	5.497	298.2	9.42	5.00	0.15	72.56
313.6	1.90	4.712	298.2	9.42	6.17	0.18	72.29
315.4	2.42	4.819	300.7	7.23	7.73	0.22	72.05
317.5	1.77	3.141	298.2	9.42	8.59	0.24	71.76
319.5	2.25	3.273	297.7	3.27	10.47	0.29	71.49
321.3	2.08	2.626	300.2	3.50	12.16	0.33	71.25
323.5	2.96	2.922	298.2	5.84	15.50	0.41	70.95
325.5	2.45	2.182	297.2	3.27	17.12	0.45	70.68
327.2	2.71	2.043	300.2	3.50	20.45	0.54	70.45
329.5	2.94	1.948	299.2	5.84	23.16	0.60	70.14
331.4	2.32	1.364	298.2	3.27	25.98	0.67	69.88
333.1	2.33	1.167	299.7	3.50	30.64	0.79	69.65
335.4	2.61	1.071	299.2	5.84	37.36	0.96	69.34
337.4	2.20	0.818	298.2	3.27	41.02	1.05	69.07
339.4	2.10	0.655	298.2	3.27	49.00	1.25	68.79
341.4	2.17	0.584	299.7	3.50	57.17	1.45	68.52
343.3	2.41	0.545	298.2	3.27	67.69	1.72	68.27
Diethylmalate: $\Delta_{vap}H^o\,(298.15\ \mathrm{K}) = (76.4 \pm 1.1)\ (\mathrm{kJ\cdot mol^{-1}})\ \ln p = \frac{396.3}{R} - \frac{118512.4}{RT} - \frac{141.2}{R}\ln\left(\frac{T}{298.15}\right)$							
313.4	3.11	10.714	296.2	8.57	3.77	0.12	74.27
315.4	3.25	9.286	295.7	8.57	4.54	0.14	73.98
317.3	2.18	5.385	296.7	4.62	5.27	0.16	73.72
319.3	3.07	6.371	296.2	6.95	6.25	0.18	73.43
321.3	3.21	5.429	295.7	8.57	7.65	0.22	73.15
323.2	2.93	4.231	296.2	4.62	8.98	0.25	72.88
325.2	3.35	4.054	296.2	6.95	10.70	0.29	72.60
327.2	3.39	3.286	295.7	8.57	13.34	0.36	72.32
329.1	3.02	2.692	296.2	4.62	14.54	0.39	72.05
331.1	3.21	2.500	296.2	3.75	16.61	0.44	71.77
333.5	3.58	2.206	294.7	5.29	20.91	0.55	71.43
335.0	2.96	1.692	296.2	4.62	22.62	0.59	71.22
337.1	2.98	1.563	296.2	3.75	24.67	0.64	70.92
339.4	3.15	1.324	295.2	5.29	30.74	0.79	70.60
340.9	4.26	1.538	296.2	4.62	35.84	0.92	70.38
343.0	3.03	1.000	295.7	3.75	39.17	1.00	70.09
345.4	3.42	0.882	295.2	5.29	49.99	1.27	69.75
346.8	6.53	1.538	296.2	4.62	54.92	1.40	69.55
348.9	3.17	0.625	295.2	3.75	65.39	1.66	69.25
351.3	5.07	0.882	295.7	5.29	74.24	1.88	68.92
353.3	21.72	3.333	295.2	8.33	84.08	2.13	68.63

Table 2. (Contd.)

T, K	m, mg	V(He), dm^3	T_a, K	Flow rate, dm^3 h^{-1}	p, Pa	$u(p)$, Pa	$\Delta_l^g H_m^o$, kJ/mol
Di-n-propylmalate: $\Delta_{vap}H^o\,(298.15\ \mathrm{K}) = (82.1 \pm 1.5)\ (\mathrm{kJ{\cdot}mol^{-1}})$ $\ln p = \frac{412.0}{R} - \frac{126996.6}{RT} - \frac{150.7}{R}\ln\left(\frac{T}{298.15}\right)$							
313.4	0.77	10.345	298.2	10.34	0.84	0.05	79.77
315.6	1.22	12.069	297.7	10.34	1.14	0.05	79.44
317.5	1.77	14.655	298.2	10.34	1.37	0.06	79.16
319.5	1.32	8.780	294.2	8.78	1.68	0.07	78.86
321.3	1.79	10.588	296.7	10.59	1.91	0.07	78.58
323.3	1.89	9.643	296.2	6.43	2.21	0.08	78.28
325.5	1.66	6.585	295.2	8.78	2.83	0.10	77.95
327.2	1.80	6.176	296.7	10.59	3.29	0.11	77.70
329.2	1.57	4.286	296.2	6.43	4.13	0.13	77.39
331.4	1.91	4.390	295.2	8.78	4.90	0.15	77.06
333.4	1.82	3.763	296.2	6.45	5.45	0.16	76.76
335.4	1.97	3.220	296.2	8.78	6.90	0.20	76.46
337.4	1.84	2.634	296.2	8.78	7.87	0.22	76.16
339.4	1.81	2.151	296.2	6.45	9.48	0.26	75.86
341.3	1.77	1.902	296.2	8.78	10.47	0.29	75.57
343.3	4.70	4.348	296.7	6.52	12.21	0.33	75.27
344.8	1.78	1.493	296.2	4.48	13.46	0.36	75.04
347.3	1.63	1.183	296.2	6.45	15.50	0.41	74.67
349.2	3.74	2.174	296.2	6.52	19.39	0.51	74.38
350.8	1.63	0.896	296.2	4.48	20.57	0.54	74.14
353.2	2.44	1.087	296.2	6.52	25.36	0.66	73.78
Di-*n*-butylmalate: $\Delta_{vap}H^o\,(298.15\ \mathrm{K}) = (89.7 \pm 1.9)\ (\mathrm{kJ{\cdot}mol^{-1}})$ $\ln p = \frac{433.7}{R} - \frac{137713.9}{RT} - \frac{161.2}{R}\ln\left(\frac{T}{298.15}\right)$							
323.5	1.18	19.091	296.2	10.91	0.62	0.02	85.57
325.3	1.05	14.754	298.2	9.84	0.72	0.02	85.28
327.3	0.98	13.793	291.2	10.35	0.70	0.02	84.96
329.5	1.49	16.071	292.2	10.71	0.92	0.03	84.61
331.2	1.50	12.500	295.2	10.71	1.20	0.03	84.33
331.5	1.55	14.285	292.2	10.71	1.07	0.03	84.28
333.2	1.26	10.056	292.2	10.06	1.24	0.03	84.01
335.5	1.47	8.928	292.2	10.71	1.63	0.04	83.64
337.1	1.73	8.929	295.2	10.71	1.93	0.05	83.38
339.2	1.47	6.704	292.2	10.06	2.17	0.06	83.04
341.3	1.65	6.364	296.2	10.91	2.60	0.07	82.70
343.3	1.71	5.556	294.2	8.33	3.05	0.08	82.38
345.1	2.00	5.555	291.2	7.41	3.55	0.09	82.09
347.4	1.82	4.018	293.2	8.04	4.50	0.11	81.72
349.3	1.88	3.472	295.2	8.33	5.40	0.14	81.41
349.3	1.94	3.571	292.2	10.71	5.36	0.14	81.41
351.2	1.57	2.459	298.2	9.84	6.44	0.16	81.11
353.2	1.78	2.425	297.2	4.16	7.35	0.19	80.79
355.2	2.00	2.222	295.2	6.67	8.99	0.23	80.46
356.7	1.70	1.705	295.2	5.11	9.94	0.25	80.22
359.1	1.53	1.386	297.2	4.16	11.11	0.28	79.83

Table 2. (End)

T, K	m, mg	V(He), dm^3	T_a, K	Flow rate, dm^3 h^{-1}	p, Pa	$u(p)$, Pa	$\Delta_l^g H_m^o$, kJ/mol
359.2	1.82	1.607	293.2	8.04	11.23	0.28	79.82
361.2	2.46	1.786	293.2	10.71	13.61	0.34	79.50
363.2	2.08	1.339	293.2	8.04	15.34	0.39	79.17
Di-*n*-pentylmalate: $\Delta_{vap}H^o(298.15\ \text{K}) = (98.0 \pm 1.0)\ (\text{kJ·mol}^{-1})$ $\ln p = \frac{457.6}{R} - \frac{149393.0}{RT} - \frac{172.4}{R}\ln\left(\frac{T}{298.15}\right)$							
329.5	0.41	17.419	298.2	11.61	0.21	0.03	92.60
331.5	0.39	14.423	298.7	11.54	0.25	0.03	92.25
333.5	0.48	13.548	298.2	11.61	0.32	0.03	91.91
335.4	0.49	11.538	298.7	11.54	0.38	0.03	91.58
337.4	0.48	9.615	298.7	11.54	0.45	0.04	91.23
339.4	0.23	3.982	298.2	7.96	0.53	0.04	90.89
341.4	0.50	6.731	299.2	11.54	0.67	0.04	90.54
343.4	0.51	5.769	299.2	11.54	0.80	0.05	90.20
345.3	0.55	5.310	298.2	7.96	0.94	0.05	89.87
347.3	0.49	3.846	299.2	11.54	1.14	0.05	89.53
348.9	0.54	3.723	299.2	6.57	1.32	0.06	89.25
351.2	0.61	3.319	298.2	7.96	1.67	0.07	88.85
353.3	0.41	1.923	299.2	11.54	1.92	0.07	88.49
354.8	0.56	2.299	299.2	6.57	2.20	0.08	88.23
357.1	0.59	1.991	298.7	7.96	2.69	0.09	87.84
359.2	0.57	1.685	299.2	6.74	3.06	0.10	87.48
360.7	0.57	1.423	299.2	6.57	3.64	0.12	87.22
363.1	0.71	1.434	298.7	6.62	4.45	0.14	86.80
365.1	0.63	1.124	299.2	6.74	5.05	0.15	86.46
367.1	0.70	1.124	299.2	6.74	5.68	0.17	86.11
369.1	0.83	1.095	299.2	6.57	6.91	0.20	85.77

Designations: T is the temperature of the study ($u(T)$ = 0.1 K), m is the mass of the transferred substance condensed at T = 228.2 K; V(He) is the volume of helium ($u(V)$ = 0.005 dm^3) used to transfer m ($u(m)$ = 0. 0001 g) of the sample; T_a is the temperature of helium flow measurement; p is the saturated vapor pressure at the temperature T; $u(p)$ is the error determined by the equation $u(p) = 0.025 + 0.025(p)$, p, Pa. The methodology for calculating the error for T, V, p, and m is given in [27].

center database [34]. The deviations of the values $\Delta_{vap}H^o$ (298.15 K) of hydroxycarboxylic acid esters and their homomorphic analogs are given in Table 3.

Analysis of the data given in Table 3 shows that the contribution to $\Delta_{vap}H^o$ (298.15 K) of the hydroxyl group and hydrogen bonding energy decreases with the increasing length of the alcoholic residue. Moreover, the contribution of hydroxyl group and hydrogen bonding energy decreases in the following sequence: glycolates – lactates – malates. This can be explained by the fact that substituents at the hydroxyl group shield the hydroxyl group and consequently decrease the hydrogen bonding energy. Shielding occurs on one side of the molecule in the case of alkyl glycolates and on both sides in the case of alkyl lactates and dialkyl malates (Fig. 5). The substituents in dialkylmalates have a larger size than the methyl substituent in alkyl lactates does and, accordingly, shielding of the hydroxyl group is greater.

In view of the above, the author's QSPR prediction method for $\Delta_{vap}H^o$ (298.15 K) and $\Delta_l^g C_{p,m}^o$ [25, 26] needed to be adjusted. Modifications were made regarding the effect of substituents on the value of the hydrogen bonding energy near the hydroxyl group, and the equation

$$\chi_b = 11.3 - \left(1.316 \cdot \ln\left({}^{0-3}\chi_{alk1} \cdot {}^{0-3}\chi_{alk2} \cdot m\right) - 0.220\right), \quad (3)$$

was obtained, where 11.3 is the hydrogen bond energy contribution from the OH-group, ${}^{0-3}\chi_{alk}$ is the total

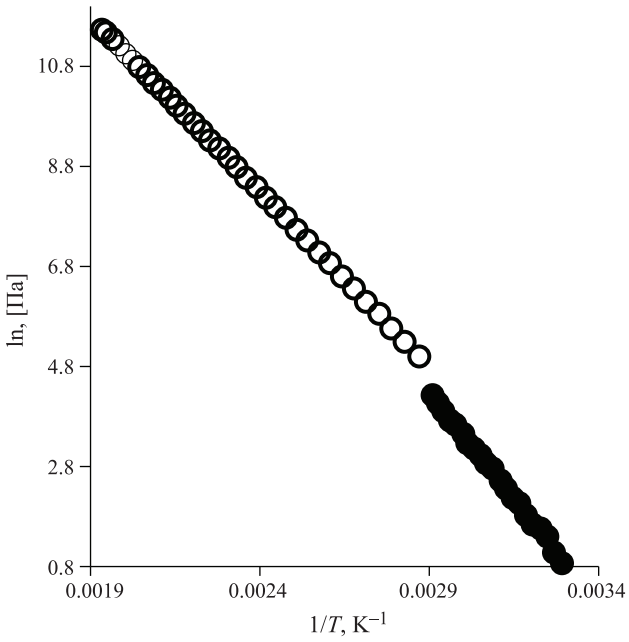


Fig. 2. Comparison of saturated vapor pressures for dimethylmalate: • this work; ○ [21].

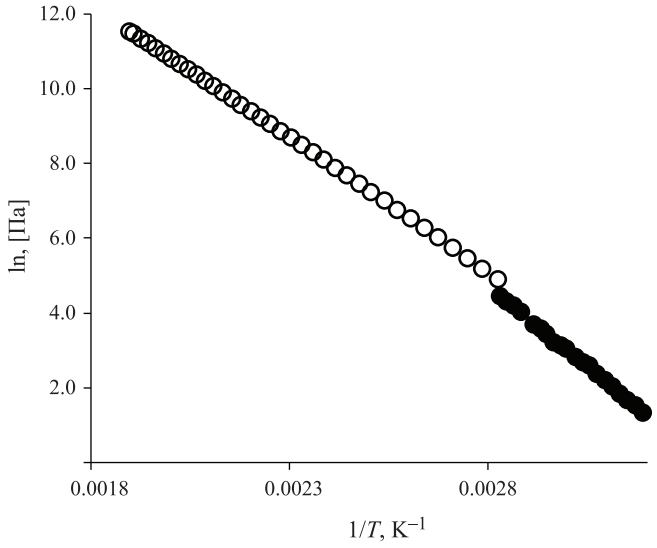


Fig. 3. Comparison of saturated vapor pressures for diethylmalate: • this work; ○ [21].

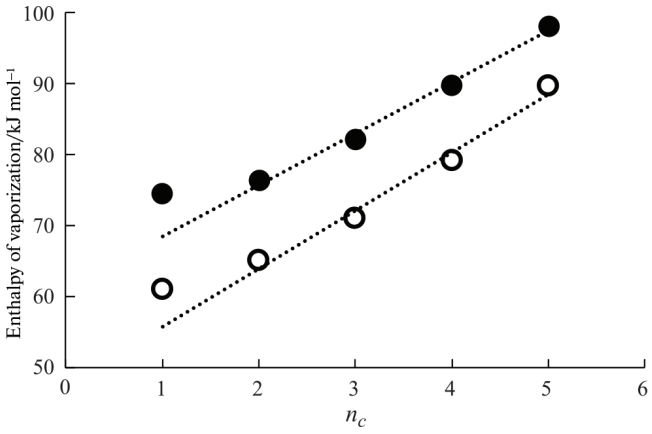


Fig. 4. Dependences of the values $\Delta_{vap}H^o$ (298.15 K) on the number of carbon atoms of the alcoholic moiety.

Table 3. Deviations (Δ) of the values $\Delta_{vap}H^o$(298.15K) of hydroxycarboxylic acid esters and their homomorphic analogs (in kJ mol^{-1}).

n_C	Δ	n_C	Δ
$\Delta_{vap}H^o$ (298.15 K) (HO-CH_2-CO_2-$(CH_2)_n$-H) – $\Delta_{vap}H^o$ (298.15 K) (CH_3-CO_2-$(CH_2)_n$-H)			
1	19.2	5	16.4
2	20.1	6	18.8
3	20.2	8	16.9
4	20.7		
$\Delta_l^g H_m^o$(298.15K) (CH_3-CH_2(OH)-CO_2-$(CH_2)_n$-H) – $\Delta_l^g H_m^o$(298.15K) (CH_3-CH_3-CO_2-$(CH_2)_n$-H)			
1	16.2	3	12.6
2	15.0	4	
$\Delta_{vap}H^o$ (298.15 K) (H-$(CH_2)_n$-CO_2-CH(OH)-CH_2-CO_2-$(CH_2)_n$-H) – $\Delta_{vap}H^o$ (298.15 K) (H-$(CH_2)_n$-CO_2-CH_2-CH_2-CO_2-$(CH_2)_n$-H)			
1	13.4	4	10.6
2	11.3	5	9.3
3	11.1		

alkane index corresponding to the substituent near the hydroxyl group (for instance, it is propane for substituent -$COOCH_2CH_3$ and butane for substituent $CH_2COOCH_2CH_3$) [25], 1.316 and 0.220 are optimization parameters. As a result, the final equation for calculating the values $\Delta_{vap}H^o$ (298.15 K) took the form

$$^{0-3}\chi = {}^0\chi + \frac{{}^1\chi}{2} + \frac{{}^2\chi}{3} + \frac{{}^3\chi}{4} + \chi_{mm} + \chi_b, \qquad (4)$$

where $^0\chi$, $^1\chi$, $^2\chi$, and $^3\chi$ are connective indices, χ_{mm} is the contribution of intermolecular interactions, and χ_b is the contribution of hydrogen bonds.

The results of calculation by the modified QSPR method are given in Table 4, which shows good convergence of the experimental and calculated data. The calculation error does not exceed 5%.

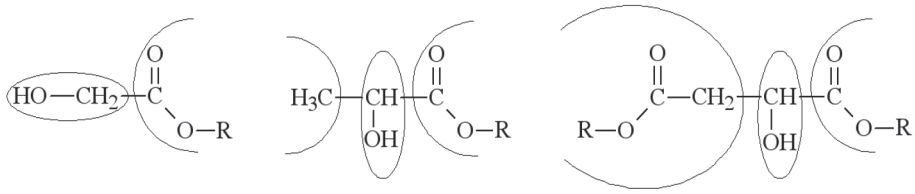


Fig. 5. Location of substituents relative to the -OH-group in molecules of alkyl glycolates, alkyl lactates, and dialkylmalates.

Table 4. Comparison of the experimental values $\Delta_{vap}H^o$ (298.15 K) in kJ mol^{-1} and calculated by the QSPR method

n_C	$\Delta_{vap}H^o$ exp.	$\Delta_{vap}H^o$ calc. (4)	n	$\Delta_{vap}H^o$ exp.	$\Delta_{vap}H^o$ calc. (4)
Alkyl glycolates					
1	52.2 ± 1.2	49.9	5	65.0 ± 1.1	65.5
2	55.1 ± 1.0	53.3	6	70.7 ± 1.3	69.5
3	58.2 ± 1.0	57.2	8	77.6 ± 2.1	78.5
4	62.7 ± 1.4	61.2			
AAPE/%					2.2
MAPE/%					4.5
Alkyl lactates					
1	50.2 ± 0.4	50.2	8	78.6 ± 1.6	79.2
2	52.8 ± 0.4	53.8	10	89.0 ± 2.2	88.4
3	56.1 ± 0.5	57.7	12	98.7 ± 3.0	97.7
4	60.2 ± 0.5	61.8	14	111.3 ± 3.8	107.1
5	64.9 ± 0.7	66.1	16	118.9 ± 3.8	116.5
6	69.7 ± 1.2	70.2			
AAPE/%					1.7
MAPE/%					3.8
Dialkylmalates					
1	74.4 ± 1.3	77.3	4	89.7 ± 1.9	88.6
2	76.4 ± 1.1	79.3	5	98.0 ± 1.0	94.7
3	82.1 ± 1.5	84.3			
AAPE/%					3.0
MAPE/%					3.9

Designations: AAPE = $(100/N)(\Sigma\left|Y_c^{\text{exp}} - Y_c^{\text{calc}}\right| / Y_c^{\text{exp}})$, where N is the number of the experimental points, Y_c^{exp} and Y_c^{calc} are the experimental and calculated values $\Delta_{vap}H^o$ (298.15 K); MAPE = $100 \cdot \left(\left|Y_c^{\text{exp}} - Y_c^{calc}\right|_{\max} / Y_c^{\text{exp}}\right)$.

FUNDING

The work was supported by the basic part of the State Assignment no. 0778-2020-0005.

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