



Determination of Antoine Constants from Estimated Vapor Pressures of Selected Food Contaminants

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Author's contribution

The sole author designed, analyzed, interpreted and prepared the manuscript.

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ABSTRACT

Aims: Accurate measurement of vapor pressure is a hard challenge in the determination of evaporation behavior of pure substances. Thus, mathematical models are widely used and are still being developed for this purpose. The aim was to tabulate Antoine constants from estimated vapor pressures of fourteen different compounds, which are mainly described as food contaminants, using property estimation software.

Study Design: Vapor pressures were estimated using an average of modified Grain–Watson and expanded Antoine methods, which are built in the preferred property estimation software. Antoine constants were calculated using linear regression and uncertainties were given in terms of standard errors of estimate.

Place and Duration of Study: The calculations were performed for two months in early 2018 and calculations took place in the Department of Food Engineering of Cankiri Karatekin University.

Methodology: Fourteen different compounds were chosen, which are all reported as liquid materials at room temperature, and temperatures for vapor pressures ranged from 298.15 K (25°C) to 473.15 K (200°C) if not exceeding normal boiling point. Vapor pressures of these compounds were estimated with property estimation software. The estimated vapor pressures were then processed using linear regression in order to create their Antoine constants with a confidence level

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of 95%. Corrected vapor pressures were calculated using their respective Antoine constants and differences were given as percentages.

Results: The maximum uncertainty was calculated as 10.5 kPa for NDMA. Calculated vapor pressures were the highest for NDMA, and the lowest for DINP. Antoine constants and calculated vapor pressures for DEP were found in accordance with previously published data found in literature.

Conclusion: Antoine constants for computational methods in the determination of vapor pressure helps to save time and effort spent on experimental methods. The outcomes of this study are thought to be useful for further studies involving computational prediction of vapor pressures of such compounds.

Keywords: Food contaminants; 3-MCPD; DEHP; Antoine constants; food safety; evaporation; food contaminants; vapor pressure.

ABBREVIATIONS

DEHP: di-2-ethylhexyl phthalate; 3-MCPD: 3-monochloro-1,2-propanediol; ATBC: acetyl tributyl citrate; DINP: di-isononylphthalate; BBP: benzyl butyl phthalate; DIBP: di-isobutyl phthalate; DEP: diethyl phthalate; DMP: dimethyl phthalate; DBS: dibutyl sebacate; DBP: dibutyl phthalate; DEHA: di-2-ethylhexyl adipate; NDMA: N-nitrosodimethylamine.

NOMENCLATURES

P^{vap}	:	Vapor pressure
ΔS_{vap}	:	Latent entropy of vaporization
R	:	Gas constant
ΔH	:	Heat of vaporization
$A, B \text{ and } C$:	Antoine constants
ΔZ_b	:	Compressibility factor
u	:	Uncertainty (expressed in standard error of estimate)

1. INTRODUCTION

Food safety has become a great concern in human diet and daily food consumption. It is now well known that contaminated foods are carrying potentially high risks for human health regardless of the way they are contaminated. Chemical, biological, physical or cross-contamination sources are the major challenges for industrial food production. Many analytical methods and devices are developed for analyzing and/or removing trace contaminants in food samples; however, it is still a problem to determine the contamination source whether from food production, food processing, or packaging [1].

It is a fact that raw food materials may already contain some chemical contaminants, such as pesticides [2,3] or heavy metals [4]. However, contamination may also occur in many steps of food processing, such as transportation, cleaning processes, heat treatment, storage and

packaging [1]. One of the most popular contaminants, 3-monochloro-1,2-propanediol (3-MCPD), is reported to form in refined vegetable oils during heat treatment [5]. N-nitrosodimethylamine (NDMA) is a semi-volatile organic compound and classified as a B2 carcinogen [6]. USEPA reports NDMA as an unintended pollutant that is released from industrial sources. It is also reported that NDMA is highly mobile in soil, which may cause leaching into drinking water [6]. 1- and 2-methylnaphthalene are both polycyclic aromatic hydrocarbons (PAH) and are reported to be potential contaminants of drinking water by dissolution in soil [7]. According to ATSDR [7], 1-methylnaphthalene is liquid while 2-methylnaphthalene is present in solid form. Like naphthalene, exposure to these chemicals is possible via outdoor air, especially around industrial areas. Another group of possible food contaminants is phthalates. Phthalates contain a vast amount of chemical compounds used as plasticizers in a wide range of plastics, including food contact materials, toys, and polyvinyl chloride (PVC) [8]. Some of these phthalates such as di-2-ethylhexyl phthalate (DEHP) are used in food packaging and are directly in contact with food materials. In addition to DEHP, the following phthalates may migrate into food material via packaging: DINP [8], BBP and DBP [9], and DIBP and DMP [10]. Some non-phthalate compounds used as phthalate alternatives including ATBC and DBS [9], DEHA [11] and 1,2-cyclohexanedicarboxylic acid,

diisononyl ester [12] are also reported as migrating contaminants to food products.

Reported techniques for the removal of phthalates are mostly based on chemical methods. Microbial degradation, oxidative processes, coagulation and adsorption on different adsorbents [13] could be given as applicable examples of these chemical removal processes. Apart from chemical methods, contaminants, including phthalates, could be separated or removed with the help of their physical properties, such as boiling point and vapor pressure. Gelmez et al. [14] reported that 98.95% reduction of initial DEHP could be achieved when molecular distillation of crude hazelnut oil was performed under 1 mbar absolute pressure at 230°C evaporation temperature. Xiong et al. [15] studied the removal of DEHP, DBP (dibutyl phthalate), and DIBP (di-isobutyl phthalate) from sweet orange oil using molecular distillation. Researchers stated that initial concentrations of 63.19 mg.kg⁻¹ for DEHP, 79.91 mg.kg⁻¹ for DBP, and 105.61 mg.kg⁻¹ for DIBP were decreased to 0.24 mg.kg⁻¹, 0.39 mg.kg⁻¹, and 0.67 mg.kg⁻¹, respectively under 50°C of evaporation temperature, 5 kPa of pressure, and 0.75 ml.min⁻¹ feeding rate.

For thermally physical separation, it is a prerequisite to know the vapor pressures of materials in subject. Precise measurement of vapor pressure is a very hard challenge especially for non-volatile compounds that have low vapor pressures. Also, adsorption of volatile compounds on equipment surfaces and the presence of impurities make sensitive measurement of vapor pressure harder [16]. In order to overcome this hurdle, vapor pressure measurement with complex and modern equipment has been studied. Hikal et al. [17] reported a method for vapor pressure measurement with UV-absorbance spectroscopy. Silva et al. [18] studied the vapor pressure determination with differential scanning calorimetry (DSC). Wu et al. [19] reported a simple method with partial saturator tubes for vapor pressure determination of various phthalates some of which are also investigated in this work. Ishak et al. [20] studied vapor pressures, aqueous solubilities and octanol-water partitions of DBP and DIBP. They used static and dynamic gas saturation methods for determining vapor pressures. Vapor pressures for numerous materials could be found in many related books and/or databases, such as Dortmund Data Bank

(<http://www.ddbst.com/ddb.html>). Alternatively, a number of equations and methods were developed in order to estimate vapor pressures at different temperatures, such as the Antoine equation, Wagner equation, Lee-Kesler method, and the Grain-Watson equation. Mohammadzadeh and Zahedi [21] proposed a new simple equation for determining vapor pressures of pure substances, which had a similar form to the Clausius-Clapeyron equation with three parameters, including critical temperature, critical pressure, and normal boiling point. Additionally, the method of Joback and Reid [22] and the method of Stein and Brown [23] are examples of some widely used group contribution methods for estimating boiling points. However, equation constants for some specific or complex compounds are not available in most books and/or databases. Therefore, the aim of this study was to compute and tabulate Antoine constants of 14 different food contaminants from their estimated vapor pressures using mathematical methods. From this point of view, this study has significance in filling the deficiency of tabulated computational constants for these compounds. Among many documents about plasticizers found in literature, only a few of them included information about their vapor pressures and estimation approaches. Therefore, the findings of this study are expected to be useful in further physical separation processes of selected food contaminants on an evaporation basis, such as molecular distillation.

2. METHODOLOGY

Vapor pressure estimations were performed on the following selected food contaminants: di-2-ethylhexyl phthalate (DEHP), 3-mono-chloro-1,2-propanediol (3-MCPD), acetyl tributyl citrate (ATBC), di-isononylphthalate (DINP), 1,2-cyclohexanedicarboxylic acid, diisononyl ester, benzyl butyl phthalate (BBP), di-isobutyl phthalate (DIBP), diethyl phthalate (DEP), dimethyl phthalate (DMP), dibutyl sebacate (DBS), dibutyl phthalate (DBP), di-2-ethylhexyl adipate (DEHA), N-nitrosodimethylamine (NDMA), and 1-methylnaphthalene. Estimations were performed using EPI-Suite v4.11 [24]. This property estimation software has three methods for estimating vapor pressure: (1) a modified version of the Grain-Watson equation [25] with a Fishtine factor [26]; (2) a derivation of the Antoine method; and (3) the Mackay method. The original Grain-Watson (GW) is given in Eq. 1.

$$\ln P^{vap} = \frac{\Delta S_{vap}}{R} \left[1 - \frac{(3 - 2T_p)^m}{T_p} - 2m(3 - 2T_p)^{m-1} \cdot \ln T_p \right] \quad (1)$$

where P^{vap} is vapor pressure in atm, ΔS_{vap} is latent entropy of vaporization, R is gas constant, $T_p = T / T_b$, $m = 0.4133 - 0.2575T_p$, and T_b and T are normal boiling point (K) and temperature (K), respectively. A simplified and widely used version of the Antoine equation and the derivation are given in Eqs. 2 and 3, respectively.

$$\ln P^{vap} = A - \frac{B}{T+C} \quad \text{or} \quad \log_{10} P^{vap} = A - \frac{B}{T+C} \quad (2)$$

$$\ln P^{vap} = \frac{\Delta H(T_b - D)^2}{\Delta Z_b R T_b^2} \left[\frac{1}{(T_b - D)} - \frac{1}{(T - D)} \right] \quad (3)$$

where ΔH is the heat of vaporization at boiling point and A, B, C and D are constants. Constant D is reported to be estimated using the formulae $D = -18 + 0.19T_b$. A compressibility factor (ΔZ_b) was used in derivations of both the GW and Antoine methods present in EPI-Suite. Compound identifiers, experimental melting points (MP), and boiling points (BP) of selected contaminants from literature were summarized in Table 1. As it can be seen from the table, all compounds were in liquid form at room temperature. Temperatures used in vapor pressure estimations ranged between 298.15 K (25°C) and 473.15 K (200°C). As it is aimed to keep compounds in liquid form for sensitive vapor pressure estimations, the maximum temperature was set to 473.15 K except for NDMA because the normal boiling point of NDMA was reported as 419.15 K (146°C).

3. RESULTS AND DISCUSSION

EPI-Suite software estimates the suggested vapor pressure as an average of modified GW and expanded Antoine method. These methods require normal boiling point (experimental-if available) for better calculations. Therefore, the experimental boiling points listed in Table 1 were provided as inputs for software. Then, vapor pressure estimations were recorded with their corresponding temperature. Linear regression with 95% confidence level was performed on these data to compute Antoine constants given in Eq. 2. using Statistica v10 (Statsoft, Tulsa, OK). Both natural (\ln) and common logarithmic (\log_{10}) forms of the Antoine equation were evaluated and computed constants are given in Table 2 with temperature units (T) in Kelvin (K) and vapor

pressures (P^{vap}) in Pascal. It should be noted that these constants would be valid for temperatures between 298.15 and 473.15 K.

Predicted vapor pressures were corrected with Antoine constants as expressed in Eq. 4. and these corrected vapor pressures ($P^{vap}_{corr.}$) were given in Table 3 along with % differences (Eq. 5).

$$P^{vap}_{corr.} = e^{\left(\frac{A-B}{T+C}\right)} \quad \text{or} \quad P^{vap}_{corr.} = 10^{\left(\frac{A-B}{T+C}\right)} \quad (4)$$

$$Difference (\%) = \left(\frac{P^{vap}_{corr.} - P^{vap}_{pre.}}{P^{vap}_{pre.}} \right) \times 100 \quad (5)$$

The comparison of corrected vapor pressures versus temperature for all contaminants in subject was given in Fig. 1. According to Fig. 1 and Table 3, NDMA had the highest vapor pressure at constant temperature which also resulted in having the lowest normal boiling point among other substances. NDMA is followed by 1-methylnaphthalene and 3-MCPD regarding their relatively higher vapor pressures at constant temperature. The highest % difference for NDMA was 0.1821% at 323.15 K. DINP had the lowest vapor pressure at all temperature values followed by DEHA. The highest % difference for DINP was calculated as 3.89% at 323.15 K.

Uncertainties (u) were also reported in Table 3 in terms of standard errors of estimate – in this case, each pressure value (P^{vap}) versus temperature (T). The highest (u) was found approximately as 10.5 kPa in NDMA. This uncertainty was thought to be a result of missing predictions because of the relatively low normal boiling point of NDMA. Also, predicted vapor pressures of NDMA were the highest among all predictions, as mentioned earlier.

As being hazardous compounds, there are a number of studies involving phthalates and their effects on health when being exposed via food package materials. General food safety rules should be obeyed while processing or during storage of food materials in contact with packaging materials that contain plasticizers. In a recent study, it was mentioned that a scandal about the illegal use of DEHP as a food additive broke out in Taiwan in May 2011 [27]. This incident also helped to raise worldwide attention to food safety. Even the effects of phthalates on human health still need to be studied thoroughly; they should be removed from foods as their presence is recognized as “contamination”.

Table 1. List of selected compounds with their melting and boiling points

Compound identifiers			Melting (MP) and Boiling (BP) Points in Literature*			
Name	IUPAC name	CAS #	Molecular formula	MP (°C)	BP (°C)	Physical state
DEHP; Di-2-ethylhexyl phthalate	bis(2-ethylhexyl) benzene-1,2-dicarboxylate	117-81-7	C ₂₄ H ₃₈ O ₄	-55 [30]	384 [30]	Liquid
3-MCPD; 3-Chloro-1,2-propanediol	3-chloropropane-1,2-diol	96-24-2	C ₃ H ₇ ClO ₂	-40 [39]	221 [30]	Liquid
ATBC; Acetyl tributyl citrate	tributyl 2-acetyloxypropane-1,2,3-tricarboxylate	77-90-7	C ₂₀ H ₃₄ O ₈	-80 [31]	173 ^{(1)*} [30]	Liquid
DINP; di-isononylphthalate	bis(7-methyloctyl) benzene-1,2-dicarboxylate	28553-12-0	C ₂₆ H ₄₂ O ₄	-43 [32]	420 [37]	Liquid
1-Methylnaphthalene	1-methylnaphthalene	90-12-0	C ₁₁ H ₁₀	-30.43 [30]	244.4 [30]	Liquid
1,2-cyclohexanedicarboxylic acid, diisononyl ester	bis(7-methyloctyl) cyclohexane-1,2-dicarboxylate	166412-78-8	C ₂₆ H ₄₈ O ₄	N/A	394 [38]	Liquid
BBP; butyl benzyl phthalate	2-O-benzyl 1-O-butyl benzene-1,2-dicarboxylate	85-68-7	C ₁₉ H ₂₀ O ₄	-35 [33]	370 [30]	Liquid
DIBP; di-iso-butyl phthalate	bis(2-methylpropyl) benzene-1,2-dicarboxylate	84-69-5	C ₁₆ H ₂₂ O ₄	-37 [34]	296.5 [30]	Liquid
DEP; diethyl phthalate	diethyl benzene-1,2-dicarboxylate	84-66-2	C ₁₂ H ₁₄ O ₄	-40.5 [30]	298 [30]	Liquid
DMP; dimethyl phthalate	dimethyl benzene-1,2-dicarboxylate	131-11-3	C ₁₀ H ₁₀ O ₄	1.03 [30]	282.7 [30]	Liquid
DBS; dibutyl sebacate	dibutyl decanedioate	109-43-3	C ₁₈ H ₃₄ O ₄	-9.2 [30]	356 [30]	Liquid
DBP; dibutyl phthalate; di-n-butyl phthalate	dibutyl benzene-1,2-dicarboxylate	84-74-2	C ₁₆ H ₂₂ O ₄	-35 [35]	340 [35]	Liquid
DEHA; di-2-ethylhexyl adipate	bis(2-ethylhexyl) hexanedioate	103-23-1	C ₂₂ H ₄₂ O ₄	-67 [36]	166-168 ^{(1)*} [36]	Liquid
NDMA; N-Nitrosodimethylamine	N,N-dimethylnitrous amide	62-75-9	C ₂ H ₆ N ₂ O	-25 (est.) [6]	146 [30]	Liquid

* Values superscripted in parentheses are reduced ambient pressures in mmHg with their corresponded boiling points. Uncertainties reported in cited references are not included

Table 2. Computed Antoine constants for selected compounds

Compound	Antoine Constants (298.15 < T < 473.15)					
	$\log_{10}(P^{vap})= A - (B / (T+C)) *$			$\ln(P^{vap})= A - (B / (T+C)) *$		
	A	B	C	A	B	C
DEHP	10.2590	3041.5065	-64.6967	23.6223	7003.3275	-64.6967
3-MCPD	10.5984	2378.907	-68.1676	24.4037	5477.636	-68.1676
ATBC	10.1328	2904.387	-67.0211	23.3317	6687.598	-67.0212
DINP	10.6968	3492.8772	-55.5240	24.6304	8042.6470	-55.5240
1-Methyl naphthalene	9.5434	2030.903	-68.8069	21.9745	4676.327	-68.8069
1,2-cyclohexane dicarboxylic acid, diisononyl ester	10.3647	3154.7415	-62.5845	23.8655	7264.0607	-62.5845
BBP	10.1244	2894.3102	-67.2003	23.3122	6664.3956	-67.2003
DIBP	9.7149	2335.1702	-70.7066	22.3695	5376.9281	-70.7066
DEP	9.7144	2340.97	-70.9445	22.3681	5390.282	-70.9445
DMP	9.6741	2256.115	-70.0274	22.2755	5194.897	-70.0274
DBS	10.0222	2769.975	-68.6364	23.0771	6378.102	-68.6364
DBP	9.9101	2632.4699	-70.2230	22.8189	6061.4859	-70.2230
DEHA	10.6598	3453.8637	-56.3030	24.5450	7952.8150	-56.3030
NDMA	9.0913	1455.642	-62.5977	20.9336	3351.739	-62.5977

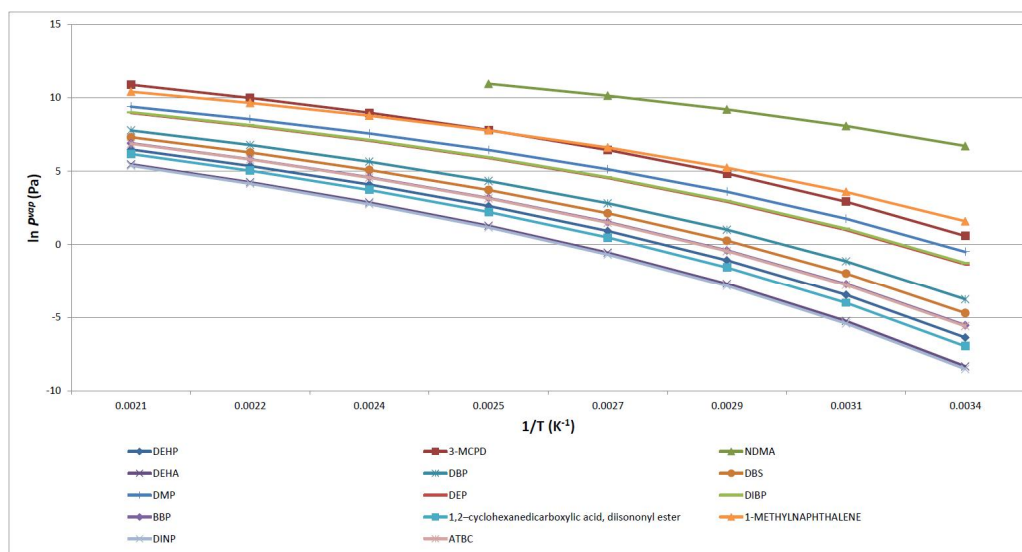
*Vapor pressure (P^{vap}) in Pa, T in K.

Fig. 1. Comparison of corrected vapor pressures versus temperature

Regarding the physical separation of these materials, there are few studies involving determining equation constants for vapor pressures of common phthalates. For instance, Roháč et al. [28] reported Antoine constants for DEP in a temperature range of 335 to 520 K, as tabulated in Table 4. Their Antoine constants were compared with this work's for a cross check at 350, 400, and 450 K. The temperatures were chosen randomly while staying in the range of both studies. According to Roháč's constants, vapor pressures were calculated as 11.74,

284.16, and 2843.95 Pa at 350, 400, and 450 K, respectively. When Antoine constants of this work were used, estimated vapor pressures were 21.16, 398.24, and 3455.89 Pa at chosen temperatures in respective order. This comparison showed a negligible difference lower than 1 kPa (0.61 kPa) between reported and estimated Antoine constants at 450 K. In another study, Berg [29] measured vapor pressures of slowly decomposing compounds, including DEP. Between temperatures of 332.211 and 452.116 K, vapor pressures of DEP reported by Berg and

Table 3. Predicted and corrected vapor pressures (P^{vap})* of selected contaminants with % differences

		Temperature (K)								$u(P^{vap})^{**}$
		298.15	323.15	348.15	373.15	398.15	423.15	448.15	473.15	
DEHP	$P^{vap}_{pre.}$	0.0017	0.0302	0.3335	2.515	13.95	60.25	213	639	160.341
	$P^{vap}_{corr.}$	0.0017	0.031	0.3379	2.5033	13.7338	59.4213	212.3948	649.5711	163.682
	<i>Diff. (%)</i>	-1.7632	2.5441	1.3316	-0.4642	-1.5501	-1.3755	-0.2841	1.6543	-
3-MCPD	$P^{vap}_{pre.}$	1.805	18.45	126	628	2460	7930	21800	52700	12236.158
	$P^{vap}_{corr.}$	1.7968	18.5643	126.3976	628.3826	2450.0543	7886.6135	21766.957	52999.228	12332.144
	<i>Diff. (%)</i>	-0.4533	0.6195	0.3156	0.0609	-0.4043	-0.5471	-0.1516	0.5678	-
NDMA***	$P^{vap}_{pre.}$	816.5	3190	9860	25400	56600	-	-	-	10473.405
	$P^{vap}_{corr.}$	815.9031	3195.8079	9855.9624	25355.2350	56661.4923	-	-	-	10505.069
	<i>Diff. (%)</i>	-0.0731	0.1821	-0.0409	-0.1762	0.1086	-	-	-	-
DEHA	$P^{vap}_{pre.}$	0.0002	0.005	0.0655	0.5785	3.685	17.95	70.3	231	59.353
	$P^{vap}_{corr.}$	0.0002	0.0052	0.0669	0.5742	3.5994	17.57	70.0571	236.6369	61.132
	<i>Diff. (%)</i>	-2.6869	3.8156	2.1783	-0.7488	-2.3223	-2.117	-0.3455	2.4402	-
DBP	$P^{vap}_{pre.}$	0.0232	0.3135	2.725	16.65	76.9	284.5	882	2360	570.993
	$P^{vap}_{corr.}$	0.0229	0.3178	2.7436	16.5964	76.2986	282.5932	880.1868	2380.9996	577.634
	<i>Diff. (%)</i>	-0.9268	1.3598	0.683	-0.3222	-0.7821	-0.6702	-0.2056	0.8898	-
DBS	$P^{vap}_{pre.}$	0.0091	0.1355	1.285	8.46	41.7	163	530	1480	363.275
	$P^{vap}_{corr.}$	0.0090	0.1377	1.2950	8.4305	41.3039	161.7309	529.0476	1494.7780	367.940
	<i>Diff. (%)</i>	-1.0842	1.6011	0.7763	-0.3488	-0.9499	-0.7786	-0.1797	0.9985	-
DMP	$P^{vap}_{pre.}$	0.611	5.735	36.35	170.5	631	1935	5105	11900	2716.226
	$P^{vap}_{corr.}$	0.6084	5.7677	36.4912	170.3021	628.4968	1927.9275	5099.2856	11954.5891	2733.579
	<i>Diff. (%)</i>	-0.4209	0.5698	0.3885	-0.1161	-0.3967	-0.3655	-0.1119	0.4587	-
DEP	$P^{vap}_{pre.}$	0.259	2.685	18.55	92.95	364.5	1175	3225	7795	1809.423
	$P^{vap}_{corr.}$	0.2577	2.7062	18.5980	92.9121	363.0145	1168.8395	3223.0786	7834.7359	1822.133
	<i>Diff. (%)</i>	-0.5186	0.7903	0.2590	-0.0408	-0.4075	-0.5243	-0.0596	0.5098	-
DIBP	$P^{vap}_{pre.}$	0.282	2.895	19.75	98.85	385	1235	3375	8130	1884.137
	$P^{vap}_{corr.}$	0.2805	2.9152	19.8696	98.6096	383.1877	1228.2158	3373.8514	8174.3621	1898.292
	<i>Diff. (%)</i>	-0.5404	0.6963	0.6058	-0.2432	-0.4707	-0.5493	-0.034	0.5457	-
BBP	$P^{vap}_{pre.}$	0.004	0.0641	0.657	4.635	24.25	99.65	337	974	241.703
	$P^{vap}_{corr.}$	0.0039	0.0655	0.6645	4.6162	23.9279	98.4326	336.3216	987.748	246.047
	<i>Diff. (%)</i>	-1.5143	2.1867	1.141	-0.4049	-1.3283	-1.2217	-0.2013	1.4115	-
1,2-cyclohexane dicarboxylic acid, diisononyl ester	$P^{vap}_{pre.}$	0.001	0.0176	0.2045	1.62	9.355	41.9	152.5	471	119.100
	$P^{vap}_{corr.}$	0.0009	0.0181	0.2076	1.6092	9.1915	41.2312	152.2431	479.4684	121.766
	<i>Diff. (%)</i>	-2.0835	3.0596	1.5341	-0.6694	-1.7482	-1.5961	-0.1685	1.798	-

		Temperature (K)								$u(P^{vap})^{**}$
		298.15	323.15	348.15	373.15	398.15	423.15	448.15	473.15	
1-Methyl naphthalene	$P^{vap}_{pre.}$	4.895	36	187	741.5	2390	6515	15500	33000	7165.609
	$P^{vap}_{corr.}$	4.8763	36.1826	187.5486	741.8646	2381.5985	6485.3884	15475.9953	33164.4661	7218.334
	$Diff.(\%)$	-0.3819	0.5073	0.2934	0.0492	-0.3515	-0.4545	-0.1549	0.4984	-
DINP	$P^{vap}_{pre.}$	0.0002	0.0043	0.0564	0.505	3.255	16.05	63.45	210	54.056
	$P^{vap}_{corr.}$	0.0002	0.0044	0.0576	0.5012	3.1798	15.6913	63.1881	215.3679	55.752
	$Diff.(\%)$	-2.7524	3.8943	2.2389	-0.7538	-2.3107	-2.2348	-0.4127	2.5562	-
ATBC	$P^{vap}_{pre.}$	0.0038	0.0608	0.6265	4.44	23.3	96.05	326	945	234.718
	$P^{vap}_{corr.}$	0.0037	0.0621	0.6334	4.4193	22.9960	94.9252	325.3378	958.1364	238.866
	$Diff.(\%)$	-1.5367	2.2634	1.0974	-0.4659	-1.3048	-1.1710	-0.2031	1.3901	-

* Vapor pressure (P^{vap}) in Pa.

** Uncertainties were expressed in terms of standard errors of estimate.

*** Reported normal boiling point for NDMA is 419.15 K (146°C)

Table 4. Comparison of Antoine constants and vapor pressures with previous work

Compound: diethyl phthalate, DEP	Comparison of Antoine constants		Comparison of vapor pressures, P^{vap} (Pa)		
	Roháč et al. [28]	This study	Temperature (K)	Berg [29]	This study*
A	22.27396	22.3681	332.211	2.69	5.68
B	5167.950	5390.282	342.187	6.23	12.13
C	-89.13509	-70.9445	352.183	13.58	24.58
Temp. range	335–520	298.15–473.15	352.197	13.52	24.60
			362.198	27.75	47.51
			372.193	54.29	87.79
			372.200	54.07	87.83
			372.219	54.24	87.93
			382.225	100.85	156.28
			392.241	182.06	268.13
			402.368	316.85	447.69
			412.380	530.31	721.27
			422.489	862.13	1135.68
			442.276	2082.3	2570.98
			452.116	3098.9	3739.76

* Calculated with computed Antoine constants (see Table 2)

this work were compared and tabulated in Table 4. The difference in vapor pressures between the two studies was found as 0.64 kPa at 452.116 K, which was also lower than 1 kPa.

4. CONCLUSION

The determination of vapor pressure for any pure substance using computational methods, such as the Antoine equation, is a beneficial way to overcome the difficulty of experimental methods. However, it could not be always possible to have the available constants required by the relevant equations. Antoine constants for different food contaminants were determined using linear regression to make vapor pressure calculations for those compounds easier. NDMA had the highest vapor pressure at all temperatures, while DINP had the lowest followed by DEHA. The maximum uncertainty in terms of standard error of estimate was approximately 10.5 kPa for NDMA. Tabulated constants from this study are thought to be useful for pre-estimations in physical separation processes, such as molecular distillation to successfully separate and/or increase the purity of target substances.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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