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Vapor Pressures, Densities, and PC-SAFT Parameters for 11 Bio-compounds

Zachariah Steven Baird[1] · Petri Uusi-Kyyny[1] · Juha-Pekka Pokki[1] · Emilie Pedegert[1] · Ville Alopaeus[1]

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Abstract
One major sustainable development goal is to produce chemicals and fuels from renewable resources, such as biomass, rather than from fossil fuels. A key part of this development is data on the properties of chemicals that appear in this bio-based supply chain. Many of the chemicals have yet to be studied thoroughly, and data on their properties is lacking. Here, we present new experimental data on the properties of 11 bio-compounds, along with PC-SAFT parameters for modeling their properties. The measured data includes vapor pressures, compressed densities, and refractive indexes. The 11 bio-compounds are tetrahydrofuran, 2-pentanone, furfural, 2-methoxy-4-methylphenol, 2-methylfuran, dihydrolevoglucosenone, cyclopentyl methyl ether, 2-*sec*-butylphenol, levoglucosenone, γ-valerolactone, and 2,6-dimethoxyphenol.

Keywords Bio-compounds · Density · PC-SAFT · Thermodynamic properties · Vapor pressure

1 Introduction

The world is increasingly searching for sustainable substitutes to replace fossil fuels. Biomass from plants is one large resource that could be converted into fuels and chemicals [1]. To accomplish this goal, some have proposed the concept of a biorefinery, which would take raw materials such as biomass and convert them into valuable products needed in modern society [2]. Similar to the current petroleum-based supply chain, a bio-based supply chain would involve hundreds of different chemicals, whether as intermediates or final products [1, 2].

✉ Petri Uusi-Kyyny
petri.uusi-kyyny@aalto.fi

[1] Department of Chemical and Metallurgical Engineering, Aalto University, P.O. Box 16100, 00076 Espoo, Finland

Chemicals relevant to the petroleum industry have been thoroughly studied over the past century, but for many bio-based chemicals there is little, if any, data about their properties. Key thermodynamic and physical properties of bio-compounds will need to be determined in order to produce bio-based chemicals. In this study we measured the vapor pressures, densities and refractive indexes of 11 such bio-compounds.

Several of these bio-compounds show up as intermediates or platform chemicals that could be further converted into a variety of products [2]. Many of the chemicals are, or could be, useful products. Dihydrolevoglucosenone is a potential bio-based alternative for dipolar aprotic solvents, such as *N*-methyl-2-pyrrolidone and dimethylformamide [3, 4]. 2,6-dimethoxyphenol has a smoky aroma and is an ingredient in artificial smoke-flavoring products [5, 6]. It, and its derivatives, could also be used for producing renewable phenolic resins [7]. 2-methoxy-4-methylphenol is used as a flavoring [8]. 2-*sec*-Butylphenol has been successfully tested as a solvent for furfural extraction in the so-called biphasic reactor concept, and it may be possible to produce it from lignin [9]. It has also been proposed that alkylphenols, such as 2-*sec*-butylphenol, be used as a solvent in biofuel production to increase the effectiveness of the process [10]. γ-valerolactone can be used as a fuel and has also been identified as a promising platform chemical that can be used to produce a variety of other chemicals [11–14]. Tetrahydrofuran is used as a solvent and in producing some polymers [15, 16]. 2-methylfuran has received attention as a potential substitute for gasoline due to its impressive combustion performance [17]. Cyclopentyl methyl ether is used as a solvent, and it has been shown to be a promising solvent for extracting compounds from the aqueous streams present in bio-refineries [18, 19]. Furfural can be used as a selective solvent and is a platform chemical that can be processed into other products [20].

Many of these compounds can also be produced from one another. For instance, dihydrolevoglucosenone is produced via hydrogenation of levoglucosenone, which itself is produced from the sugar levoglucosan that is formed in the pyrolysis of lignocellulosic biomass [21]. In addition, there are reactions for converting between 2-methylfuran, tetrahydrofuran, furfural, and 2-pentanone [2, 22]. 1,3-dimethoxy-2-hydroxybenzene and 2-methoxy-4-methylphenol have been found in plants and in pyrolysis oil [23].

For 6 (2-methoxy-4-methylphenol, 2-*sec*-butylphenol, 2,6-dimethoxyphenol, cyclopentyl methyl ether, dihydrolevoglucosenone, levoglucosenone) of the 11 compounds there is only a small amount of data, if any at all. For 5 bio-compounds (2-methylfuran, 2-pentanone, furfural, tetrahydrofuran, γ-valerolactone) large amounts of data can be found in the literature. However, even for these 5 compounds the data presented here extends beyond the range covered in the literature. For 7 of the bio-compounds (2-methoxy-4-methylphenol, 2-methylfuran, 2-pentanone, cyclopentyl methyl ether, dihydrolevoglucosenone, furfural, tetrahydrofuran) we measured compressed densities at higher pressures (up to 12 or 16 MPa), and for many of the compounds there was no reliable data available at higher pressures. We have placed a file containing both the literature data we found and our experimental data in a repository at the Open Science Framework,

and this file can be obtained at (https://osf.io/u9amn/). An overview of the measurements made in this work is presented in Table 1.

2 Methods

2.1 Chemicals

Information about the chemicals used in this study is presented in Tables 2 and 3. The structures of the chemicals are presented in Fig. 1 [24]. The purities were measured using gas chromatography with a flame ionization detector. For most of the chemicals the water content was also measured using a DL38 Karl Fischer Titrator (Mettler Toledo). The purity was calculated by taking the relative peak area from

Table 1 Overview of the measurements made in this work

Name	Measured property	Measurement temperature, K	Measurement pressure, MPa
2-Methoxy-4-methylphenol	Density, liquid	293.15–473.15	0.12–11.85
	Vapor pressure, liquid	298.22–403.2	9.3E−6–5.3E−3
	Refractive index, liquid	293.15–343.15	0.1
2-Methylfuran	Density, liquid	293.14–473.16	0.09–11.85
	Refractive index, liquid	293.15	0.1
2-Pentanone	Density, liquid	293.15–473.16	0.09–11.85
	Refractive index, liquid	293.15	0.1
2-*sec*-Butylphenol	Density, liquid	293.15–473.16	0.101
	Vapor pressure, liquid	298.21–403.25	4.7E−6–4.6E−3
	refractive index, liquid	293.15–343.15	0.1
2,6-Dimethoxyphenol	Density, liquid	333.16–383.16	0.1
	Vapor pressure, liquid	333.28–413.16	1.4E−5–1.9E−3
	Refractive index, liquid	328.15–343.15	0.1
Cyclopentyl methyl ether	Density, liquid	293.14–473.15	0.09–11.85
Dihydrolevoglucosenone	Density, liquid	293.15–423.16	0.07–15.77
	Vapor pressure, liquid	298.26–403.16	1.4E−5–5.2E−3
	Refractive index, liquid	293.15–343.15	0.1
Furfural	Density, liquid	293.15–448.15	0.09–11.9
Levoglucosenone	Density, liquid	293.15–363.15	0.1
	Vapor pressure, liquid	298.26–403.3	6.2E−6–3.5E−3
	Refractive index, liquid	293.15–343.15	0.1
Tetrahydrofuran	Density, liquid	293.14–473.15	0.1–11.85
	Refractive index, liquid	293.15	0.1
γ-Valerolactone	Vapor pressure, Liquid	298.23–403.15	4.4E−5–9.9E−3
	Refractive index, liquid	293.15–333.15	0.1

Table 2 Names, identifiers, and suppliers of the chemicals used in this study

Name	Other names	CAS number	InChI key	Supplier
2-Methoxy-4-methylphenol	Creosol, 4-methylguaiacol	93-51-6	PETRWTHZSKVLRE-UHFFFAOYSA-N	Sigma-Aldrich
2-Methylfuran		534-22-5	VQKFNUFAXTZWDK-UHFFFAOYSA-N	Sigma-Aldrich
2-Pentanone	Methyl propyl ketone	107-87-9	XNLICIUVMPYHGG-UHFFFAOYSA-N	Sigma-Aldrich
2-*sec*-Butylphenol	*o*-*sec*-Butylphenol	89-72-5	NGFPWHGISWUQOI-UHFFFAOYSA-N	Sigma-Aldrich
2,6-Dimethoxyphenol	Syringol	91-10-1	KLIDCXVFHGNTTM-UHFFFAOYSA-N	Sigma-Aldrich
Cyclopentyl methyl ether	Methoxycyclopentane	5614-37-9	SKTCDJAMAYNROS-UHFFFAOYSA-N	Sigma-Aldrich
Dihydrolevoglucosenone	Cyrene; (5 ~ {*R*})-6,8-dioxabicyclo[3.2.1]octan-4-one	53716-82-8	WHIRALQRTSITMI-BAFYGKSASA-N	Circa
Furfural	Furan-2-carbaldehyde	98-01-1	DIHRNGWBOKYHHW-UHFFFAOYSA-N	Sigma-Aldrich
Levoglucosenone	(1 ~ {*S*},5 ~ {*R*})-6,8-dioxabicyclo[3.2.1]oct-2-en-4-one	37112-31-5	HITOXZPZGPXYHY-UJURSFKZSA-N	Circa
Tetrahydrofuran	Oxolane	109-99-9	WYURNTSHIVDZCO-UHFFFAOYSA-N	Merck
γ-Valerolactone	5-Methyldihydrofuran-2(3H)-one; 5-methyloxolan-2-one	108-29-2	GAEKPEKOJKCEMS-UHFFFAOYSA-N	SAFC

Table 3 Purities of the chemicals used in this study

Name	Purification method	Water content (wt%)	Purity (wt%)	Refractive index nD (at 293 K)[a]
2-Methoxy-4-methylphenol		0.39	99.4	1.5373
2-Methylfuran	Distillation	0.015	99.9	1.4332
2-Pentanone		0.05	99.8	1.3903
2-*sec*-Butylphenol	Vacuum distillation		99.9	1.5228
2,6-Dimethoxyphenol			99.7	
Cyclopentyl methyl ether		0.0027	100.0	
Dihydrolevoglucosenone		0.045	99.8	1.4732
Furfural	Vacuum distillation	0.013	99.8	
Levoglucosenone			96.2	1.5064
Levoglucosenone	Vacuum distillation	0.25	98.7	1.5065
Tetrahydrofuran		0.033	99.9	1.4073
γ-Valerolactone	Vacuum distillation		99.5	1.4333

[a]Atmospheric pressure 0.10 ± 0.01 MPa

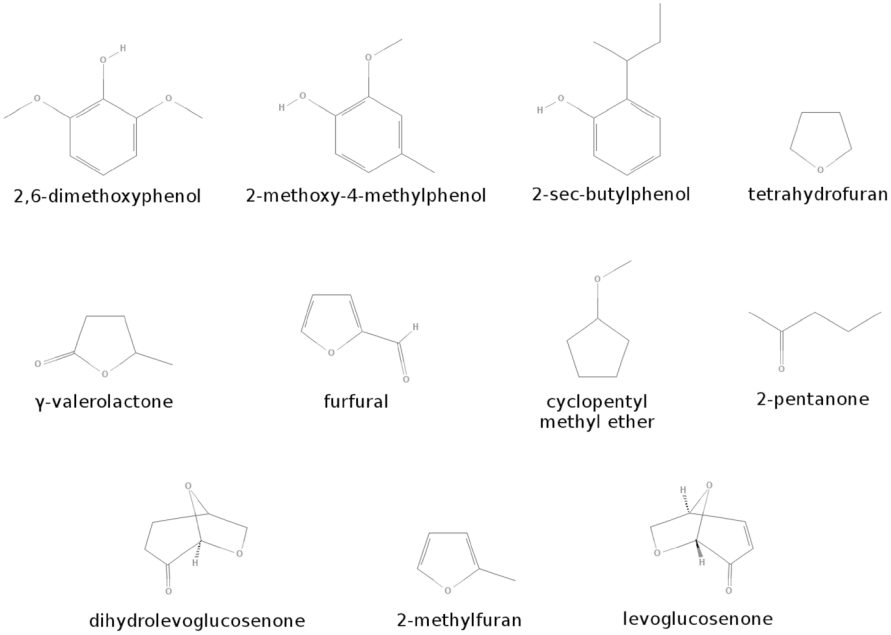

Fig. 1 Structures of the chemicals measured in this study. Structures were obtained from PubChem [24]

the chromatogram and then accounting for any water by dividing by 1 plus the water content (if measured).

All samples except one had purities close to 100 %. The one exception was the levoglucosenone used for vapor pressure measurements, which only had a purity of 96.2 wt%. Mass spectroscopy was used to investigate what impurities were present, and most of them were lower weight impurities such as 2-methylpentane, hexane, methylcyclopentane, cyclohexane and acetone. The levoglucosenone also contained one heavier impurity: 2-methoxyphenol. These impurities could be tolerated when measuring the vapor pressure because in the gas saturation method most of the light impurities are removed in the first run. This occurred with levoglucosenone in this study: the vapor pressure was much higher for the first run, and that point was removed. After the vapor pressure measurement, the purity of the levoglucosenone condensed at the outlet of the gas saturation cell was determined to be 98.5 wt%. Later the levoglucosenone was distilled to get a higher purity for the density and refractive index measurements. This distilled sample had a purity of 98.7 wt%.

2.2 Density Measurements

Densities were measured with a DMA HP density meter (Anton Paar). Most of the samples were measured at a range of pressures, and for these measurements a UNIK 5000 pressure sensor (GE) was used (range of 0 to 20 MPa, abs.). The sensor had been calibrated against a MC2-PE calibrator with an EXT600 external pressure module (Beamex). The MC2-PE calibrator had been calibrated by Beamex. The pressure data has a standard uncertainty of 3100 Pa (expanded uncertainty of 6300 Pa at the 95 % level). For three of the samples measurements were only made at atmospheric pressure, and pressure data were taken from the Finnish Meteorological Institute (Tapiola observation station, Espoo, Finland) [25]. For the temperature, the manufacturer of the density meter only states that the accuracy is better than 0.1 K.

The samples were degassed for about 30 min before measuring. This was done by placing the sample in a round-bottomed flask, which was then placed in an ultrasonic bath. Gasses were removed from the system using a vacuum pump.

Water and nitrogen were used to calibrate the density meter. Reference values for these compounds were taken from reference equations of state, [26, 27] and we used the implementations of these equations available in the CoolProp package for Python [28]. Alternatively, these equations of state are also implemented in the NIST thermophysical properties calculator, [29] and we verified the CoolProp implementation by manually comparing the results of the two programs at multiple temperatures and pressures. For optimizing the calibration equation parameters we used the differential evolution solver [30] implemented in the SciPy package [31] for Python. The root mean-squared error between the reference and calculated values was used as the objective function.

Between samples, the performance of the device was checked by measuring air and water. During the study the performance checks indicated that a recalibration was necessary, so for later samples, a second set of calibration parameters were used.

For the first calibration the standard uncertainty was estimated to be 0.047 kg·m^{-3} (expanded uncertainty of 0.092 kg·m^{-3} at the 95 % level). For the second calibration, the standard uncertainty was estimated to be 0.036 kg·m^{-3} (expanded uncertainty of 0.072 kg·m^{-3} at the 95 % level). One major uncertainty component of density is the impurities in the sample. The impurities are sample specific and the effect is included in the uncertainty estimates given in the density results.

One sample, levoglucosenone, was measured at atmospheric pressure using a DMA 5000 M density meter (Anton Paar). The performance of the device was checked with water and air, and based on this the expanded uncertainty at the 95 % level was estimated to be 0.05 kg·m^{-3}.

Bio-compounds are often thermally unstable. The densities of decomposition products often deviate from that of the pure measured component. In some cases, this allows potential decomposition to be detected by just observing density changes during the measurement. When measuring furfural, decomposition was observed at 473 K. Dihydrolevoglucosenone started to react at 423 K. The density value was stable for about the first 20 min at this temperature, but then started to increase. Therefore, the few points from the beginning of the measurement at 423 K are included in the data file, but these points were not included during regression.

2.3 Gas Saturation Measurements

A gas saturation method was used to measure the vapor pressures of 6 of the bio-compounds (2-methoxy-4-methylphenol, 2-*sec*-Butylphenol, 2,6-dimethoxyphenol, dihydrolevoglucosenone, levoglucosenone, and γ-valerolactone. About 10 ml of each sample was placed in a glass vessel filled with spherical glass beads, and the vessel was put in a gas chromatography oven. The oven maintained a stable temperature (fluctuations were within ± 0.01 K). A flow of nitrogen was introduced, and this gas became saturated with the vaporized compound. To maintain the flow rate of nitrogen, a flow controller (Alicat Scientific, Tucson, AZ, USA) was placed in the nitrogen inlet line. The nitrogen flow rate was measured with a bubble meter, both before and after each run (standard uncertainty of 0.039 ml·min^{-1}, expanded uncertainty of 0.088 ml·min^{-1} at the 95 % level). The vessel was left in the oven for a period of time (on the order of hours). Afterwards, it was removed and weighed to determine the mass lost. The vapor pressure was then calculated based on Eq. 1

$$P = \frac{\frac{m}{W}}{\left(\frac{m}{W} + \frac{tVP_{atm}}{T_{room}R}\right)} \cdot \left(P_{atm} + \Delta P_{loss}\right) \tag{1}$$

where P is the vapor pressure (Pa), m is the mass of the test chemical that leaves the cell (g), W is the molar mass of the test chemical (g·mol^{-1}), t is the duration of the measurement (min), V is the volumetric flow rate of the carrier gas (in this case, nitrogen) in units of L·min^{-1}, P_{atm} is the atmospheric pressure at the place and time the experiment is carried out (Pa), T_{room} is room temperature (K), R is the ideal gas constant, and ΔP_{loss} is the pressure drop over the gas saturation cell (assumed to be

zero for our measurements). More details about the gas saturation method can be found from other references [32, 33].

Atmospheric pressure was taken from values measured by the Finnish Meteorological Institute (Tapiola observation station, Espoo, Finland) [25]. The cell and room temperatures were measured with calibrated Pt-100 temperature probes (Frontec) connected to a Systemteknik S2541 thermometer (Frontec). These probes had an expanded uncertainty of 0.04 K (using a coverage factor of 2).

The uncertainty of the vapor pressures were calculated using a Monte Carlo method (see ISO/IEC Guide 98-3) [34]. 8 different parameters were included that could potentially affect the vapor pressure value, including the purity of each compound. The uncertainty of those 8 parameters was used to specify a distribution for each, and values were then selected from those distributions to calculate a vapor pressure value. This was repeated 1 million times for each experimental data point. The standard uncertainty of each vapor pressure point was taken to be the standard deviation of the distribution from the Monte Carlo calculation. The calculated uncertainties can be found in the vapor pressure data file in the OSF project for this article (https://osf.io/u9amn/). The code we used for performing the uncertainty calculations can also be found in the same OSF project (https://osf.io/u9amn/).

2.4 Refractive Index Measurements

Refractive indexes were measured using a Dr. Kernchen Abbemat digital refractometer (Anton Paar, Graz, Austria), and this refractometer measures at a wavelength of 598.3 nm. Based on measurements with water at 25 °C, the standard uncertainty of the refractometer was calculated to be 0.00 034 (expanded uncertainty of 0.00 078 at the 95 % level). Reference data for water were obtained from Schiebener et al. [35].

2.5 Modeling with PC-SAFT

The PC-SAFT equation of state was used to model the properties of the bio-compounds [36]. Because all of the bio-compounds contain polar and/or associating functional groups, contributions from the dipole and associating terms were also included, as appropriate [37–42]. When including the dipole term from Gross and Vrabec, the equation is also called the PCP-SAFT equation of state [38].

De Villiers et al. [43] showed that it can be difficult to find the best fit for polar compounds using pure component data alone. Often there is a large range of parameter values that will give good results for pure component properties, but poor results for mixtures. De Villiers et al. suggested that this could be because it is difficult to disentangle the contribution from polar interactions from the part due to dispersion forces. They proposed including VLE data with a nonpolar component when fitting the pure component parameters for polar compounds. Because such data is not available for many of the bio-compounds studied in this article, we simply set the number of dipoles (a parameter in Gross and Vrabec's dipole term) equal to the actual number of polar functional groups in the molecule. This was the same strategy originally proposed by Gross and Vrabec [38]. The one exception was for furfural. A good fit

could not be achieved unless the number of dipoles was also fitted against experimental data.

The dipole term also uses the dipole moment of the compound as a parameter. For most of the bio-compounds, the dipole moments were found in the literature [44–49]. Levoglucosenone was the only compound for which the dipole moment could not be found. Therefore, for use as a parameter in the PC-SAFT equation, the dipole moment was set to be equal to that of dihydrolevoglucosenone, since they are structurally similar compounds.

For some of the compounds in this article PC-SAFT parameters have already been presented in the literature (2-methylfuran, [50, 51]; 2-pentanone [37, 52]; cyclopentyl methyl ether [53]; furfural [37, 54]; tetrahydrofuran [37, 55] and γ-valerolactone [56]. We have refit parameters for these compounds because we had more data to include in the regression, including the new data measured in this article. Both literature data and data from this study were used when optimizing the PC-SAFT parameters. A file containing all the data used in optimization, including references, can be obtained from the OSF page (https://osf.io/u9amn/). It should be noted that in the data from Apaev et al. [57] for 2-pentanone there seems to have been a typo for the point at 376.63 K and 687 bar (probably should have been 799.5 instead of 899.5 $kg \cdot m^{-3}$), and we made this change in our literature data file. The total number of points used in the optimization and the number of literature data points is presented in Table 4. A total of 969 new measured data points were used in the regression.

Parameters were optimized by minimizing the root mean-squared errors of the vapor pressure and density added together. Optimization was performed using the differential evolution solver implemented in the Scipy package for Python [30, 31]. The resulting PC-SAFT parameters are given in Table 3. Our code for implementing the PC-SAFT equation of state can be found on GitHub: https://github.com/zmeri/PC-SAFT.

3 Results and Discussion

3.1 Compressed Liquid Density, Liquid Vapor Pressure and Refractive Index Measurement Results

The results for the density measurement are presented in Tables 5, 6, 7, 8, 9, 10, 11, 12, 13 and 14. The results for the vapor pressure measurement are presented in Tables 15, 16, 17, 18, 19 and 20. The measurements of the refractive index of the components can be found in Table 21.

3.2 Comparison with Literature Values

A lot of literature data is available for tetrahydrofuran, and our experimental density values matched well with most of the literature values. For instance, at 293.15 K the value we measured was close to the mean of the literature data (see Table 22) and

Table 4 PC-SAFT parameters obtained for the 11 bio-compounds

Compound	m	σ	ε/k	μ	n_m	κ^{AB}	ε^{AB}/k	Density, ARD (%)	Vapor press., ARD (%)	Temp. range (K)	Nr. points used	Nr. lit. points
2-Methoxy-4-methylphenol	4.0723	3.5395	291.48	2.83	1	0.091 033	1017.8	0.084	6.0	288–494	192	5
2-Methylfuran	2.8077	3.4608	253.86	0.72	1	–	–	0.36	1.4	251–516	442	316
2-Pentanone	3.2373	3.5126	251.25	2.77	1	–	–	0.13	0.90	199–539	537	408
2-*sec*-Butylphenol	4.3601	3.6800	292.29	–	–	3.2993×10^{-6}	3940.1	0.65	5.8	293–501	28	2
2,6-Dimethoxyphenol	4.5567	3.4499	299.94	2.10	2	0.075,030	1270.7	0.013	2.1	333–535	18	2
Cyclopentyl methyl ether	2.9310	3.7553	272.93	1.27	1	–	–	0.31	0.53	278–473	153	27
Dihydrolevoglucosenone	3.7546	3.3705	264.85	3.4	3	–	–	0.94	3.3	293–403	76	2
Furfural	3.5218	3.1933	291.71	3.60	0.371	–	–	0.090	1.8	251–527	332	211
Levoglucosenone	4.2036	3.1804	254.72	3.4[a]	3	–	–	0.69	7.8	293–403	27	0
Tetrahydrofuran	2.4371	3.5195	275.90	1.75	1	–	–	0.13	0.57	213–533	887	763
γ-Valerolactone	3.1504	3.4996	313.05	4.30	1	–	–	0.20	2.0	238–480	240	227

m is the segment number, σ is the segment diameter (Å), ε/k is the dispersion energy divided by the Boltzmann constant (K), μ is the dipole moment, n_μ is the number of dipole moments, κ^{AB} is the association volume, ε^{AB}/k is the association energy divided by the Boltzmann constant (K), and ARD is average relative deviation

[a]No dipole moment could be found in the literature for levoglucosenone, so for the PC-SAFT equation the dipole moment of dihydrolevoglucosenone was used

Table 5 Compressed liquid density of 2-methoxy-4-methylphenol (creosol)

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
0.940	298.15	1092.38	1.025	433.16	962.89
0.444	298.15	1092.14	0.527	433.15	962.10
1.914	298.15	1092.96	0.144	433.15	961.62
3.900	298.15	1094.10	1.509	433.15	963.22
5.886	298.15	1095.18	2.005	433.14	963.80
7.869	298.15	1096.19	2.501	433.15	964.34
9.852	298.15	1097.24	2.996	433.15	964.90
11.832	298.15	1098.23	3.493	433.15	965.46
0.943	323.16	1069.03	3.989	433.15	966.01
0.446	323.16	1068.70	4.487	433.15	966.52
1.931	323.15	1069.66	4.982	433.15	967.09
3.915	323.15	1070.89	5.478	433.14	967.66
5.900	323.15	1072.11	5.974	433.15	968.16
7.885	323.15	1073.27	1.035	433.15	962.66
9.866	323.15	1074.46	1.019	413.14	982.66
11.846	323.15	1075.60	0.536	413.14	982.20
0.955	323.15	1069.04	0.135	413.15	981.75
1.011	333.15	1059.62	1.510	413.15	983.16
0.515	333.15	1059.29	2.004	413.14	983.64
0.120	333.15	1059.04	2.499	413.14	984.16
1.500	333.15	1059.96	2.997	413.15	984.65
1.997	333.15	1060.29	3.492	413.15	985.12
2.490	333.15	1060.62	3.990	413.15	985.63
2.989	333.15	1060.95	4.485	413.15	986.10
3.483	333.15	1061.28	4.984	413.14	986.63
3.980	333.15	1061.61	5.480	413.14	987.09
4.476	333.15	1061.89	5.976	413.14	987.61
4.975	333.15	1062.22	1.030	413.15	982.64
5.471	333.15	1062.55	1.028	298.15	1092.76
5.967	333.15	1062.88	0.540	298.15	1092.48
1.011	333.15	1059.67	0.145	298.15	1092.27
1.030	293.15	1097.17	1.514	298.15	1093.06
0.538	293.15	1096.88	2.011	298.15	1093.34
0.135	293.15	1096.63	2.506	298.15	1093.63
1.512	293.15	1097.51	3.003	298.15	1093.87
2.009	293.15	1097.75	3.499	298.15	1094.15
2.504	293.15	1098.04	3.996	298.15	1094.44
3.003	293.15	1098.28	4.490	298.15	1094.72
3.497	293.15	1098.56	4.988	298.15	1094.95
3.994	293.15	1098.80	5.485	298.15	1095.23
3.993	293.15	1098.75	5.981	298.15	1095.52
4.490	293.15	1099.03	1.040	298.15	1092.77

Table 5 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
4.988	293.15	1099.26	0.536	393.14	1001.91
5.485	293.15	1099.54	0.144	393.14	1001.52
5.982	293.15	1099.83	1.020	393.14	1002.33
1.037	293.15	1097.12	1.510	393.14	1002.80
1.038	313.16	1078.42	2.007	393.15	1003.21
0.543	313.16	1078.14	2.503	393.15	1003.68
0.134	313.15	1077.84	3.002	393.15	1004.10
1.511	313.15	1078.72	3.496	393.15	1004.52
1.511	313.15	1078.72	3.992	393.14	1005.00
2.008	313.15	1079.01	4.488	393.14	1005.42
2.504	313.15	1079.29	5.482	393.14	1006.31
3.001	313.15	1079.63	4.987	393.14	1005.84
3.497	313.15	1079.91	5.978	393.14	1006.73
3.994	313.15	1080.19	1.032	393.15	1002.32
4.488	313.15	1080.48	0.531	453.16	942.46
4.989	313.15	1080.76	0.144	453.16	941.94
5.483	313.15	1081.09	1.017	453.16	943.11
5.980	313.15	1081.37	1.510	453.16	943.71
1.040	313.15	1078.38	2.007	453.15	944.38
1.022	353.16	1040.71	2.502	453.15	944.98
0.540	353.16	1040.33	2.997	453.16	945.62
0.135	353.15	1040.04	3.494	453.16	946.27
1.510	353.15	1041.04	3.991	453.16	946.87
2.006	353.15	1041.42	4.486	453.16	947.48
2.503	353.15	1041.80	4.985	453.16	948.08
3.001	353.15	1042.13	5.481	453.16	948.69
3.497	353.15	1042.51	5.975	453.15	949.30
3.991	353.15	1042.84	1.036	453.15	943.13
4.489	353.15	1043.21	1.019	473.16	922.11
4.987	353.15	1043.59	0.537	473.15	921.38
5.483	353.15	1043.92	1.032	473.15	922.41
5.980	353.15	1044.24	1.512	473.16	922.95
1.034	353.15	1040.67	2.007	473.15	923.65
1.017	373.16	1021.60	2.501	473.15	924.39
0.533	373.16	1021.17	2.999	473.15	925.09
0.133	373.15	1020.84	3.495	473.15	925.78
1.510	373.15	1021.98	3.993	473.15	926.53
2.007	373.15	1022.41	4.487	473.15	927.17
2.503	373.15	1022.78	4.986	473.15	927.87
2.999	373.15	1023.20	5.481	473.15	928.57
3.496	373.16	1023.57	5.977	473.15	929.27

Table 5 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
3.992	373.15	1023.96	0.538	473.15	921.53
4.489	373.15	1024.34	1.030	473.15	922.46
4.986	373.15	1024.76			
5.481	373.15	1025.13			
5.977	373.15	1025.55			
1.031	373.15	1021.56			

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.66 kg·m^{-3} (expanded uncertainty of 1.3 kg·m^{-3} at the 95 % level)

was well within the standard deviation of the literature values (0.33 kg·m^{-3}, with outliers removed).

We found seven literature sources that give compressed densities of tetrahydrofuran, and when comparing we found that the data from many of these literature sources seems to have relatively large errors [58–64]. Figure 2 compares the literature sources and values from this article, using the PC-SAFT fit for tetrahydrofuran as a reference. The points from Holzapfel et al. [58] and Sato et al. [59] aligned well with our data, as did much of the data from Govender et al. [60]. Data from Vasileva et al. [61] was in the same range as our data, but in general the deviations between the two data sets were larger than the measurement uncertainty of our data. The largest difference is 12 kg·m^{-3}, and this occurs at 473.15 K and about 21 bar. At 293.15 K the value from Vasileva et al. is more than 7 standard deviations higher than the literature mean, and so it seems that there is a higher uncertainty in the data from Vasileva et al. The vapor pressures from Vasileva et al. also had some of the largest deviations from the PC-SAFT equation.

The data from the other three sources [62–64] was significantly lower than our values and those from other literature sources. Although these researchers mostly measured at much higher pressures than the other sources, values at atmospheric pressure show that these three data sets have significant errors. For instance, at 323.15 K and atmospheric pressure the value from Schornack and Eckert [62] is more than 35 standard deviations below the mean of the other literature values (ours was within a standard deviation). There may have been some problem with their experimental setup because their value for chlorobenzene at 323 K and atmospheric pressure is 10 kg·m^{-3} lower than the value from the DIPPR correlation [45], so there seems to be a consistent negative deviation. Zhang and Kiran [63] did not measure at atmospheric pressure, but extrapolating from their data down to atmospheric pressure using a linear pressure dependency shows a similar large negative deviation from most other literature sources. The uncertainty caused by the extrapolation is in this case a magnitude lower than the deviation.

Table 6 Compressed liquid density of 2-Methylfuran

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
0.495	298.14	909.96	5.922	373.15	823.16
0.095	298.14	909.46	6.912	373.15	824.89
0.989	298.14	910.40	7.899	373.15	826.62
1.974	298.14	911.38	8.885	373.15	828.29
2.963	298.14	912.40	9.872	373.15	829.92
3.952	298.14	913.42	10.856	373.15	831.50
4.940	298.14	914.39	11.842	373.15	833.12
5.929	298.14	915.36	1.004	398.15	777.14
6.916	298.14	916.32	0.612	398.15	776.12
7.904	298.14	917.28	1.973	398.16	779.62
8.891	298.14	918.25	2.961	398.16	782.07
9.877	298.14	919.16	3.946	398.16	784.46
10.860	298.14	920.11	4.936	398.15	786.82
11.847	298.14	921.02	5.924	398.15	789.07
0.500	293.15	915.84	6.912	398.15	791.32
0.088	293.14	915.46	7.898	398.15	793.47
0.995	293.15	916.39	8.887	398.15	795.57
1.972	293.15	917.36	9.874	398.16	797.61
2.960	293.15	918.33	10.859	398.16	799.62
3.949	293.15	919.30	11.843	398.16	801.52
4.938	293.15	920.22	1.001	298.16	910.52
5.926	293.15	921.19	0.989	423.15	736.05
6.913	293.15	922.11	11.848	423.14	768.03
7.899	293.15	923.02	11.845	423.14	768.38
8.886	293.15	923.93	10.881	423.15	766.03
9.874	293.15	924.85	11.843	423.15	768.37
10.858	293.15	925.75	9.898	423.15	763.51
11.843	293.15	926.61	8.918	423.15	760.94
0.508	323.16	879.22	7.934	423.16	758.25
0.092	323.15	878.68	6.948	423.16	755.49
0.986	323.15	879.81	5.963	423.16	752.58
11.847	323.15	892.53	4.967	423.15	749.60
10.882	323.15	891.48	3.982	423.15	746.50
9.902	323.15	890.43	2.990	423.15	743.21
8.921	323.15	889.33	2.001	423.16	739.81
7.935	323.15	888.22	1.005	423.16	736.18
6.951	323.15	887.07	1.009	423.15	736.15
5.959	323.15	885.91	11.843	423.15	768.40
4.977	323.15	884.75	1.583	448.15	691.16
3.984	323.15	883.55	11.844	448.14	733.04
2.994	323.15	882.34	10.867	448.15	729.98
1.998	323.15	881.12	9.895	448.15	726.76

Table 6 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
0.512	348.15	847.10	8.916	448.15	723.39
11.845	348.15	863.31	7.931	448.15	719.79
10.879	348.15	862.07	6.947	448.15	716.05
9.896	348.15	860.78	5.956	448.14	712.07
8.916	348.15	859.44	4.974	448.15	707.93
7.933	348.15	858.09	3.982	448.15	703.52
6.948	348.15	856.75	2.992	448.15	698.73
5.961	348.15	855.31	2.000	448.14	693.56
4.971	348.15	853.91	1.597	448.15	691.36
3.976	348.15	852.42	2.277	473.15	637.03
2.993	348.15	850.97	10.878	473.15	690.57
1.995	348.15	849.42	11.843	473.15	694.63
1.006	348.15	847.88	9.898	473.15	686.19
0.212	348.15	846.65	8.910	473.14	681.52
0.505	373.15	812.92	7.933	473.16	676.50
0.406	373.15	812.69	6.947	473.15	671.08
0.985	373.15	813.84	5.961	473.15	665.28
1.971	373.15	815.77	4.969	473.15	658.86
2.958	373.15	817.69	3.982	473.15	651.78
3.946	373.15	819.52	2.990	473.15	643.66
4.935	373.15	821.34	2.287	473.15	637.22

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.11 kg·m^{-3} (expanded uncertainty of 0.21 kg·m^{-3} at the 95 % level)

For instance, at 302.4 K we got a value of 848.2 kg·m^{-3} when extrapolating their data, which is about 28 kg·m^{-3} lower than the literature mean.

For the vapor pressure measurements gamma-valerolactone could be used as a reference compound for validating our gas saturation method. We found the literature data from 11 other sources, and we compared these different data sets in Fig. 3 [56, 65–74]. Most of the data fall within a few percentage points of each other, but there is one point from Havasi et al. [69] that is about 40 % lower than the other data. It is so far out of line that it is below the y-axis limits in Fig. 3. In general, the data from Havasi et al. show an increasing negative deviation at lower temperatures, which could indicate a problem with the measurement procedure at those temperatures. The 3 points at the lowest temperatures from Havasi et al. were left out when fitting the PC-SAFT parameters.

Table 7 Compressed liquid density of 2-pentanone

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.495	298.14	801.70	7.900	373.15	736.41
0.095	298.14	801.35	8.889	373.15	737.74
0.987	298.15	802.14	9.874	373.15	739.02
1.973	298.15	803.01	10.859	373.15	740.25
2.962	298.15	803.87	11.845	373.15	741.48
3.951	298.15	804.74	0.496	298.15	801.74
4.939	298.15	805.56	0.492	398.16	697.96
5.926	298.15	806.42	0.305	398.16	697.60
6.917	298.15	807.23	11.847	398.16	717.17
7.903	298.15	808.05	10.869	398.15	715.75
8.890	298.15	808.86	9.905	398.15	714.30
9.877	298.15	809.62	8.923	398.15	712.78
10.862	298.15	810.43	7.941	398.15	711.22
11.845	298.15	811.18	6.953	398.15	709.56
0.497	293.15	806.56	5.965	398.15	707.89
0.091	293.15	806.21	4.979	398.15	706.18
0.986	293.15	806.95	3.987	398.15	704.43
1.973	293.15	807.82	2.995	398.15	702.68
2.962	293.15	808.64	2.004	398.15	700.88
3.949	293.15	809.46	1.011	398.15	698.97
4.940	293.15	810.28	0.999	423.15	669.40
5.927	293.15	811.09	0.515	423.16	668.10
6.915	293.15	811.86	11.848	423.15	692.13
7.902	293.15	812.67	10.883	423.15	690.43
8.889	293.15	813.44	9.903	423.14	688.59
9.874	293.15	814.20	8.920	423.15	686.69
10.860	293.15	814.96	7.938	423.15	684.75
11.844	293.15	815.71	6.951	423.14	682.79
0.509	323.16	777.26	5.966	423.14	680.75
0.086	323.15	776.82	4.979	423.15	678.61
0.987	323.15	777.75	3.986	423.15	676.39
1.973	323.15	778.81	2.997	423.15	674.17
2.961	323.15	779.82	2.003	423.14	671.87
3.949	323.15	780.83	1.005	423.14	669.41
4.940	323.15	781.79	0.987	448.16	636.76
5.927	323.15	782.80	0.754	448.16	635.93
6.914	323.15	783.75	11.847	448.15	665.96
7.901	323.15	784.71	10.879	448.16	663.78
8.889	323.15	785.66	9.903	448.16	661.56
9.875	323.15	786.56	8.919	448.16	659.21
10.859	323.15	787.47	7.937	448.16	656.81
11.845	323.15	788.37	6.952	448.15	654.33

Table 7 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.512	348.15	752.02	5.957	448.15	651.75
0.086	348.15	751.49	4.976	448.16	649.05
0.985	348.15	752.60	3.977	448.16	646.18
1.972	348.15	753.85	2.993	448.16	643.21
2.959	348.15	755.05	2.003	448.15	640.12
3.948	348.15	756.24	1.010	448.15	636.87
4.939	348.15	757.44	1.099	473.16	600.03
5.925	348.15	758.59	11.849	473.15	638.34
6.913	348.15	759.73	9.899	473.15	632.90
7.902	348.15	760.87	7.939	473.15	626.90
8.888	348.15	761.97	5.965	473.15	620.25
9.876	348.15	763.06	3.986	473.14	612.91
10.858	348.15	764.15	1.997	473.15	604.46
11.845	348.15	765.20	1.104	473.15	600.13
0.502	373.15	725.68	1.101	473.15	600.09
0.114	373.15	725.04	2.961	473.15	608.54
0.987	373.15	726.44	4.936	473.15	616.46
1.972	373.15	727.92	6.913	473.14	623.50
2.959	373.15	729.40	8.889	473.16	629.85
3.948	373.15	730.84	10.859	473.15	635.67
4.938	373.15	732.27	1.107	473.15	600.13
5.925	373.15	733.70	0.496	298.15	801.73
6.914	373.15	735.08			

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.21 $kg \cdot m^{-3}$ (expanded uncertainty of 0.41 $kg \cdot m^{-3}$ at the 95 % level)

Our data falls in line with the literature data, although it has a somewhat larger scatter than some of the literature data sets. In more recent experiments with the gas saturation equipment, we were able to improve the repeatability by making repeat measurements of the cell mass and taking the average of them, [75] so it seems that uncertainty in the sample weight was the largest contribution to the uncertainty for the gas saturation measurements presented here. We did not observe any systematic bias in our data when compared to the model or other data.

Table 8 Liquid density of 2-*sec*-butylphenol at atmospheric pressure

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.102	293.15	981.32
0.103	298.14	977.22
0.103	298.16	977.25
0.103	313.16	965.03
0.103	333.16	948.54
0.103	353.16	931.70
0.103	373.16	914.64
0.103	393.15	897.29
0.103	413.16	879.65
0.103	433.16	861.73
0.103	453.15	843.35
0.103	473.16	824.44

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.11 $kg \cdot m^{-3}$ (expanded uncertainty of 0.22 $kg \cdot m^{-3}$ at the 95 % level)

Table 9 Liquid density of 2,6-dimethoxyphenol (syringol) at atmospheric pressure

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg\ m^{-3}$)[c]
0.101	333.16	1158.57
0.101	343.16	1148.88
0.101	353.16	1139.15
0.101	363.15	1129.40
0.101	373.16	1119.48
0.101	383.16	1109.63

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.30 $kg \cdot m^{-3}$ (expanded uncertainty of 0.60 $kg \cdot m^{-3}$ at the 95 % level)

3.3 Results and PC-SAFT Modeling

The data accompanying this article has been uploaded to a scientific repository (Open Science Framework), and it can be accessed at https://osf.io/u9amn/. The repository contains the density, vapor pressure, and refractive index data. Here, we give an overview of the results.

Table 10 Compressed liquid density of cyclopentyl methyl ether

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.505	298.14	858.52	5.926	373.15	790.28
0.099	298.15	858.12	6.915	373.15	791.61
0.990	298.15	858.91	7.900	373.15	792.89
1.979	298.14	859.73	8.889	373.15	794.18
2.965	298.14	860.56	9.876	373.15	795.41
3.956	298.14	861.38	10.859	373.15	796.64
4.943	298.14	862.20	11.845	373.15	797.83
5.931	298.14	863.01	0.512	398.15	755.18
6.920	298.14	863.78	0.310	398.15	754.82
7.907	298.14	864.54	0.988	398.15	756.04
8.894	298.14	865.35	1.973	398.15	757.80
9.882	298.14	866.11	2.959	398.15	759.56
10.867	298.14	866.87	3.950	398.15	761.22
11.851	298.14	867.58	4.940	398.15	762.84
0.514	293.14	863.31	5.927	398.15	764.46
0.098	293.15	862.95	6.916	398.15	766.08
0.988	293.15	863.69	7.902	398.15	767.59
11.853	293.15	872.11	8.890	398.15	769.16
10.886	293.15	871.40	9.876	398.15	770.62
9.908	293.15	870.69	10.860	398.15	772.04
8.927	293.15	869.98	11.845	398.15	773.46
7.940	293.15	869.22	0.496	298.15	858.51
6.955	293.15	868.45	1.002	423.15	726.95
5.969	293.15	867.69	0.506	423.16	725.80
4.977	293.15	866.92	11.851	423.16	748.37
3.982	293.15	866.15	10.889	423.15	746.73
3.000	293.15	865.33	9.909	423.15	744.99
2.003	293.15	864.56	8.921	423.15	743.19
0.513	323.16	834.09	7.943	423.16	741.38
0.097	323.15	833.70	6.959	423.16	739.49
0.988	323.15	834.58	5.964	423.16	737.54
1.974	323.15	835.55	4.983	423.15	735.57
2.962	323.15	836.56	3.987	423.15	733.54
3.951	323.15	837.52	2.997	423.15	731.41
4.942	323.15	838.43	2.002	423.16	729.21
5.926	323.15	839.39	0.700	448.15	694.30
6.916	323.15	840.30	11.852	448.15	722.29
7.902	323.15	841.20	10.890	448.14	720.28
8.889	323.15	842.11	9.906	448.14	718.20
9.876	323.15	843.01	8.927	448.15	716.02
10.861	323.15	843.92	7.944	448.15	713.76
11.844	323.15	844.77	6.957	448.15	711.40

Table 10 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.509	348.15	808.94	5.968	448.15	708.95
0.092	348.15	808.41	4.982	448.15	706.45
0.987	348.15	809.47	3.983	448.14	703.81
11.852	348.15	821.55	2.997	448.15	701.12
10.886	348.15	820.55	1.996	448.15	698.29
9.905	348.15	819.56	1.010	448.15	695.32
8.920	348.15	818.51	0.710	448.15	694.40
7.942	348.15	817.42	11.851	473.14	694.93
6.955	348.15	816.37	1.506	473.15	661.90
5.963	348.15	815.27	1.011	473.15	659.73
4.980	348.15	814.17	1.980	473.15	663.68
3.986	348.15	813.02	2.965	473.15	667.54
2.994	348.15	811.87	3.951	473.15	671.20
2.004	348.15	810.73	4.940	473.15	674.68
0.513	373.16	782.72	5.928	473.15	677.96
0.107	373.16	782.14	6.916	473.15	681.07
0.988	373.16	783.44	7.904	473.15	684.07
1.971	373.16	784.83	8.889	473.15	686.99
2.964	373.16	786.27	9.877	473.15	689.76
3.948	373.15	787.60	10.861	473.15	692.39
4.940	373.15	788.99	11.846	473.15	694.97

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.10 kg m^{-3} (expanded uncertainty of 0.20 kg m^{-3} at the 95 % level)

Table 22 gives the density at 293 K for each of the 10 compounds measured in this study. Literature values are also given for comparison, where available. In general, our measured results match well with literature values. However, with 2-methoxy-4-methylphenol and 2-*sec*-butylphenol there are relatively large discrepancies between the experimental and literature values [75–101]. For both of these compounds only one literature value could be found, and they were from articles in 1952 and 1896 that used methods with higher uncertainties. The value for 2-pentanone may also seem to be out of line at first glance; however, when looking at the individual literature values one can see large variations between the different sources [82–100]. There are 5 sources that give a density close to ours (about 806.3 $kg \cdot m^{-3}$), but 6 of the 19 sources give a higher density of about 809 $kg \cdot m^{-3}$. So many of the values actually lie more than 1 $kg \cdot m^{-3}$ away from the mean. It is unclear why there is such a large scatter in the data for 2-pentanone, although all of the highest values

Table 11 Compressed liquid density of dihydrolevoglucosenone

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.090	293.15	1250.75	15.756	348.15	1207.18
3.943	293.15	1252.88	0.088	348.15	1196.86
9.868	293.15	1256.00	1.953	348.15	1198.15
13.804	293.15	1257.92	3.930	348.15	1199.47
15.764	293.15	1258.89	5.907	348.15	1200.83
5.919	293.15	1253.91	7.882	348.15	1202.14
7.894	293.15	1254.94	5.906	373.15	1176.75
11.837	293.15	1256.99	1.978	373.15	1173.80
1.967	293.15	1251.77	3.928	373.15	1175.25
0.093	298.15	1245.77	7.881	373.15	1178.24
0.984	298.15	1246.32	0.086	373.15	1172.28
9.872	298.15	1251.16	9.856	373.15	1179.67
13.808	298.15	1253.14	11.824	373.15	1181.11
15.768	298.15	1254.11	13.791	373.15	1182.49
1.947	298.15	1246.95	15.754	373.15	1183.87
1.948	298.15	1247.00	1.952	373.16	1173.74
1.969	298.15	1246.85	5.902	398.15	1152.51
3.946	298.15	1247.95	7.879	398.15	1154.19
5.923	298.15	1249.03	9.852	398.15	1155.82
7.897	298.15	1250.10	11.823	398.15	1157.44
11.843	298.15	1252.16	13.789	398.15	1159.02
0.084	323.15	1221.30	15.749	398.15	1160.55
1.957	323.15	1222.51	1.976	398.15	1149.35
3.933	323.15	1223.70	3.926	398.15	1150.87
5.912	323.15	1224.92	1.949	398.16	1149.14
7.886	323.15	1226.08	0.082	398.16	1147.60
9.860	323.15	1227.24	1.958	423.15	1124.40
11.830	323.15	1228.38	0.073	423.14	1122.74
13.795	323.15	1229.51	0.091	423.15	1122.77
15.760	323.15	1230.58	1.950	423.16	1124.38
9.856	348.15	1203.43	15.756	423.16	1137.14
11.827	348.15	1204.67	9.888	423.14	1131.94
13.792	348.15	1205.96	1.971	423.14	1124.61

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.25 $kg \cdot m^{-3}$ (expanded uncertainty of 0.51 $kg \cdot m^{-3}$ at the 95 % level)

Table 12 Compressed liquid density of furfural

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.497	293.15	1160.04	1.974	373.15	1074.66
0.092	293.15	1159.79	2.959	373.15	1075.61
0.987	293.15	1160.38	3.949	373.15	1076.51
1.973	293.15	1161.01	4.940	373.15	1077.41
2.961	293.15	1161.64	5.929	373.15	1078.35
3.950	293.15	1162.22	6.916	373.15	1079.25
4.940	293.15	1162.84	7.903	373.15	1080.14
5.930	293.15	1163.46	8.890	373.15	1080.99
6.920	293.15	1164.07	9.878	373.15	1081.88
7.905	293.15	1164.64	10.863	373.15	1082.73
8.894	293.15	1165.24	11.849	373.15	1083.57
9.881	293.15	1165.85	0.510	373.15	1073.27
10.865	293.15	1166.40	0.495	398.16	1044.93
11.851	293.15	1167.00	0.092	398.16	1044.54
0.495	298.14	1154.82	0.987	398.15	1045.45
0.093	298.14	1154.52	11.856	398.15	1056.72
0.988	298.15	1155.06	10.874	398.15	1055.78
1.973	298.15	1155.69	9.894	398.15	1054.84
2.962	298.15	1156.32	8.912	398.15	1053.80
3.952	298.15	1156.99	7.928	398.15	1052.78
4.941	298.15	1157.61	6.942	398.15	1051.79
5.929	298.15	1158.23	5.954	398.15	1050.80
6.917	298.15	1158.84	4.966	398.15	1049.76
7.904	298.15	1159.45	3.974	398.15	1048.73
8.893	298.15	1160.06	2.983	398.15	1047.64
9.878	298.15	1160.67	1.990	398.15	1046.59
10.864	298.15	1161.27	0.518	398.15	1044.99
11.849	298.15	1161.82	0.494	423.16	1015.70
0.514	298.15	1154.81	0.108	423.14	1015.20
0.499	298.15	1154.81	0.986	423.14	1016.34
0.496	323.15	1128.08	11.854	423.14	1029.37
0.089	323.15	1127.78	9.892	423.15	1027.14
0.986	323.15	1128.47	7.925	423.15	1024.83
1.974	323.15	1129.14	5.953	423.14	1022.50
2.962	323.15	1129.86	3.975	423.14	1020.10
3.951	323.15	1130.53	0.515	423.15	1015.76
4.940	323.15	1131.24	1.976	423.15	1017.54
5.929	323.15	1131.96	2.964	423.15	1018.77
6.917	323.15	1132.62	4.941	423.14	1021.23
7.903	323.15	1133.32	6.917	423.14	1023.63
8.890	323.15	1133.98	8.891	423.15	1025.96
9.878	323.15	1134.68	10.863	423.15	1028.22

Table 12 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
10.862	323.15	1135.33	0.514	423.16	1015.74
11.850	323.15	1135.98	0.491	448.15	985.23
0.495	348.16	1100.92	0.298	448.14	984.99
0.087	348.15	1100.58	11.852	448.15	1001.25
0.988	348.15	1101.31	9.891	448.15	998.65
1.971	348.15	1102.12	7.924	448.15	996.02
2.961	348.15	1102.93	5.951	448.15	993.24
3.950	348.15	1103.74	3.970	448.15	990.43
4.940	348.15	1104.55	1.987	448.14	987.54
5.928	348.15	1105.31	0.514	448.15	985.33
6.917	348.15	1106.11	0.513	448.15	985.28
7.904	348.15	1106.91	0.988	448.14	986.04
8.891	348.15	1107.66	2.962	448.15	988.93
9.879	348.15	1108.41	4.940	448.15	991.79
10.863	348.15	1109.16	6.917	448.15	994.56
11.849	348.15	1109.91	8.892	448.15	997.29
0.500	373.16	1073.32	10.863	448.14	999.94
0.091	373.15	1072.93	0.509	448.15	985.37
0.988	373.16	1073.70			

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.24 $kg \cdot m^{-3}$ (expanded uncertainty of 0.47 $kg \cdot m^{-3}$ at the 95 % level)

were measured more than 50 years ago, and the more recent articles report a lower density.

Using the PC-SAFT equation, we could calculate the normal boiling point (at 101,325 Pa) and enthalpy of vaporization of each compound. These values are given in Table 23. For dihydrolevoglucosenone and levoglucosenone the PC-SAFT equation had to be extrapolated about 100 K above the available vapor pressure data to reach the boiling point, so the boiling points for these compounds contain larger uncertainty. For dihydrolevoglucosenone Sherwood et al. [3] measured an approximate value of 476 K for the boiling point using a TGA, which is about 20 K lower than the value we calculated. We observed that dihydrolevoglucosenone decomposed even at 423 K (see Sect. 2.2), and so it is possible that decomposition occurred in the TGA measurement, leading to an estimated value lower than the actual boiling point.

We can also briefly examine the relationships between molecular structure and properties. For instance we can see that hydrogenating levoglucosenone to

Table 13 Liquid density of levoglucosenone

Pressure (MPa)[a]	Temperature (K)[b]	Density (kg m^{-3})[c]
0.100	293.15	1303.6
0.100	298.15	1298.6
0.100	313.15	1283.5
0.100	328.15	1268.4
0.100	343.15	1253.3
0.100	353.15	1243.3
0.100	363.15	1233.2
0.100	293.15	1303.6
0.100	298.15	1298.6
0.100	313.15	1283.5
0.100	328.15	1268.4
0.100	343.15	1253.3
0.100	353.15	1243.3
0.100	363.15	1233.2
0.100	298.15	1298.6

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 1.7 kg·m^{-3} (expanded uncertainty of 3.4 kg·m^{-3} at the 95 % level)

dihydrolevoglucosenone gives a compound with a somewhat lower vapor pressure and density. This may be useful information in designing processes that produce dihydrolevoglucosenone from levoglucosenone. γ-valerolactone also stands out because it has a much higher boiling point than other compounds with similar molar masses.

4 Conclusions

Vapor pressures, densities, and refractive indexes were measured for a group of bio-compounds. For several of the compounds this is the first publicly available data on these properties. The experimental data measured here showed good agreement with most literature data for tetrahydrofuran and γ-valerolactone. Comparison also showed that density data at higher pressures from several of the literature sources was erroneous, both for tetrahydrofuran and for 2-pentanone. The new density data in this article helps to fill the gaps left when removing those unreliable datasets.

Table 14 Compressed liquid density of tetrahydrofuran

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
0.402	298.15	882.38	9.901	348.15	837.19
0.099	298.15	882.02	8.920	348.15	836.10
0.992	298.15	882.81	7.933	348.15	834.96
11.854	298.15	891.84	6.953	348.15	833.81
10.874	298.15	891.09	5.962	348.15	832.61
9.893	298.15	890.29	4.979	348.15	831.47
8.909	298.15	889.53	3.987	348.15	830.22
7.925	298.15	888.73	2.997	348.15	829.02
6.941	298.15	887.92	2.006	348.15	827.77
5.954	298.15	887.11	0.215	348.15	825.49
4.965	298.15	886.24	0.988	373.15	796.10
3.977	298.15	885.42	1.974	373.16	797.63
2.986	298.15	884.55	2.960	373.15	799.18
1.994	298.15	883.68	3.948	373.15	800.67
0.513	298.15	882.42	4.937	373.15	802.14
0.502	293.15	887.82	5.925	373.15	803.62
0.111	293.15	887.47	6.910	373.15	805.06
11.854	293.15	896.95	7.898	373.15	806.44
0.494	293.15	887.77	8.886	373.15	807.82
11.854	293.15	896.96	9.874	373.15	809.20
10.892	293.15	896.25	10.857	373.15	810.53
9.910	293.15	895.50	11.842	373.15	811.81
1.013	293.14	888.32	0.512	373.15	795.44
1.986	293.15	889.09	0.313	373.15	795.02
2.968	293.15	889.92	0.500	398.16	762.57
3.953	293.15	890.74	1.974	398.15	765.55
4.940	293.15	891.56	11.848	398.15	783.16
5.928	293.15	892.37	10.867	398.15	781.60
6.917	293.15	893.14	9.898	398.15	780.08
7.904	293.15	893.95	8.916	398.16	778.41
8.890	293.15	894.70	7.933	398.16	776.74
0.512	323.15	854.73	6.943	398.16	774.98
0.103	323.15	854.29	5.965	398.15	773.22
0.986	323.15	855.22	4.975	398.15	771.41
11.852	323.15	865.93	3.985	398.15	769.55
10.885	323.15	865.03	2.995	398.15	767.65
9.905	323.15	864.13	1.007	398.16	763.67
8.924	323.15	863.18	0.899	423.15	727.70
7.940	323.15	862.23	0.990	423.16	727.96
6.949	323.15	861.28	11.847	423.16	753.18
5.970	323.15	860.32	2.002	423.15	730.83
4.978	323.15	859.32	2.969	423.16	733.24
3.987	323.15	858.31	3.954	423.16	735.70

Table 14 (continued)

Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]	Pressure (MPa)[a]	Temperature (K)[b]	Density ($kg \cdot m^{-3}$)[c]
3.001	323.15	857.30	4.940	423.16	738.08
2.002	323.15	856.28	5.929	423.15	740.47
1.998	443.14	699.53	6.914	423.15	742.75
2.972	443.14	702.90	7.901	423.15	744.94
11.849	443.15	727.80	8.886	423.16	747.10
3.986	443.15	706.29	9.879	423.16	749.19
4.957	443.15	709.28	10.857	423.15	751.20
5.940	443.15	712.17	2.094	473.16	644.15
6.925	443.15	715.01	11.846	473.15	686.73
7.909	443.14	717.78	10.872	473.15	683.48
8.895	443.15	720.41	9.898	473.15	680.08
9.880	443.15	722.97	8.910	473.15	676.45
10.865	443.15	725.44	7.932	473.15	672.68
1.393	443.15	697.40	6.948	473.15	668.67
1.017	298.15	882.85	5.961	473.15	664.38
0.509	348.15	825.84	4.975	473.15	659.81
0.992	348.15	826.47	3.982	473.15	654.91
11.846	348.15	839.27	2.985	473.15	649.50
10.882	348.15	838.28	2.494	473.15	646.62

[a]The standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)

[b]Standard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)

[c]Standard uncertainty of the density is 0.1 $kg \cdot m^{-3}$ (expanded uncertainty of 0.2 $kg \cdot m^{-3}$ at the 95 % level)

Table 15 Vapor pressure of liquid 2-methoxy-4-methylphenol

Temperature K[a]	Vapor pressure Liquid Pa	Expanded uncertainty of vapor pressure at 95 % level Pa
298.22	9.3	1.0
303.24	16.1	1.4
313.25	31.7	3.0
323.24	81.8	6.4
323.25	82.1	6.2
333.27	143.0	6.3
343.22	274.5	9.2
353.27	476	20
363.22	807	42
373.21	1533	58
383.22	2280	119
393.16	3520	122
403.20	5320	141

[a]Standard uncertainty of the temperature u(T) = 0.04 K

Table 16 Vapor pressure of liquid 2-*sec*-butylphenol

Temperature K[a]	Vapor pressure liquid (Pa)	Expanded uncertainty of vapor pressure at 95 % level (Pa)
298.21	4.74	0.74
303.24	8.5	1.3
313.25	18.4	2.5
323.25	49.4	5.5
333.29	94.2	11
343.23	231	24
343.24	226.6	6.9
353.28	449	23
363.23	663	21
363.26	659	35
373.25	1097	60
383.31	1868	96
393.25	2940	126
403.25	4570	139

[a]Standard uncertainty of the temperature u(T) = 0.04 K

Table 17 Vapor pressure of liquid 2,6-dimethoxyphenol (syringol)

Temperature K[a]	Vapor pressure liquid (Pa)	Expanded uncertainty of vapor pressure at 95 % level (Pa)
333.28	15.8	1.5
333.30	14.3	2.0
343.22	31.7	1.8
353.27	64.0	6.0
363.25	122.3	2.8
373.24	233	10
383.28	401	24
393.25	722	32
403.26	1123	42
413.16	1884	64

[a]Standard uncertainty of the temperature u(T) = 0.04 K

Table 18 Vapor pressure of liquid Dihydrolevoglucosenone (cyrene)

Temperature K[a]	Vapor pressure liquid (Pa)	Expanded uncertainty of vapor pressure at 95 % level (Pa)
298.26	14.4	2.4
308.31	28.2	2.5
318.24	51.5	8.0
328.27	116.9	6.1
333.32	157.3	7.0
338.27	219.4	7.4
343.26	294	15
343.26	288	12
353.25	506.1	7.1
363.26	842	29
373.24	1324	69
378.23	1780	111
383.26	2133	93
393.18	3490	202
403.16	5170	229

*Standard uncertainty of the temperature u(T) = 0.04 K

Table 19 Vapor pressure of liquid Levoglucosenone

Temperature (K)[a]	Vapor pressure liquid (Pa)	Expanded uncertainty of vapor pressure at 95 % level (Pa)
298.26	6.2	1.7
303.25	10.0	2.3
313.26	26.0	4.6
323.25	42.2	7.8
333.29	90.3	8.6
343.24	205	11
353.26	374	28
363.27	621	36
373.27	909	57
383.29	1502	85
393.26	2450	122
403.30	3480	137

[a]Standard uncertainty of the temperature u(T) = 0.04 K

Table 20 Vapor pressure of liquid γ-valerolactone

Temperature (K)[a]	Vapor pressure liquid (Pa)	Expanded uncertainty of vapor pressure at 95 % level (Pa)
298.23	43.6	3.1
303.20	64.8	3.2
313.25	136.7	7.0
323.25	244	12
333.29	453	21
343.18	763	22
343.28	791	38
353.26	1293	29
363.25	2060	61
373.17	3120	173
383.12	2280	144
393.08	3520	223
403.15	5320	346

[a]Standard uncertainty of the temperature u(T) = 0.04 K

Table 21 Refractive index of liquid Dihydrolevoglucosenone (cyrene), γ-valerolactone, 2-methoxy-4-methylphenol (creosol), 2-*sec*-butylphenol, Levoglucosenone, 2,6-dimethoxyphenol (syringol), Tetrahydrofuran, 2-pentanone, 2-methylfuran at 0.10 MPa

Temperature K[a]	Refractive index[b]								
	Dihydrolevo-glucosenone (cyrene)	γ-Valerolactone	2-Methoxy-4-methylphenol (creosol)	2-*sec*-Butyl-phenol	Levoglucose-none	2,6-Dimeth-oxyphenol (syringol)	Tetrahydro-furan	2-Pentanone	2-Methylfuran
293.15	1.4732	1.4333	1.5373	1.5228	1.5065		1.4073	1.3903	1.4332
298.15	1.4712	1.4313	1.5348	1.5205					
303.15	1.4691	1.4292	1.5323	1.5171	1.5022				
308.15	1.4671	1.4272	1.5299	1.5146					
313.15	1.4651	1.4252	1.5274	1.5113	1.4980				
318.15	1.4631	1.4231	1.525	1.5086					
323.15	1.4611	1.4211	1.5225	1.5062	1.4938				
328.15	1.4592	1.4191	1.5200	1.5039		1.5365			
333.15	1.4571	1.4170	1.5176	1.5018	1.4896	1.5344			
338.15			1.5151	1.5000		1.5320			
343.15			1.5126	1.4980	1.4854	1.5296			

Standard uncertainty of the pressure is 0.01 MPa

[a]Standard uncertainty of the temperature is 0.03 K

[b]Standard uncertainty of liquid refractive index: u(refractive index) = 0.00 034, (expanded uncertainty of 0.00 078 at the 95 % level)

Table 22 Comparison of experimental density values from this study with literature values

Compound	Density at 293.15 K ($kg \cdot m^{-3}$)		References
	This work	Literature[a]	
2-Methoxy-4-methylphenol	1096.6 ± 1.3	1090.05	[76]
2-Methylfuran	915.46 ± 0.1	915.31 ± 0.48	[77–81]
2-Pentanone	806.21 ± 0.41	807.80 ± 0.56	[82–100]
2-*sec*-Butylphenol	977.24 ± 0.22[b]	980.4[b]	[101]
2,6-Dimethoxyphenol	1158.57 ± 0.6[c]	–	
Cyclopentyl methyl ether	862.95 ± 0.2	862.80 860.43	[102] [103]
Dihydrolevoglucosenone	1250.75 ± 0.51	1250 1251.7	[3] [44]
Furfural	1159.79 ± 0.47	1160.10 ± 0.45	[79, 93, 104–113]
Levoglucosenone	1303.6 ± 3.4	–	
Tetrahydrofuran	887.47 ± 0.2	887.57 ± 0.14	[58, 114–129]
γ-Valerolactone	–	1054.61 ± 1.4	[56, 67, 68, 130–132]

[a]Mean of literature values, if more than two literature values were available and outliers were removed

[b]At 298.15 K

[c]At 333.16 K

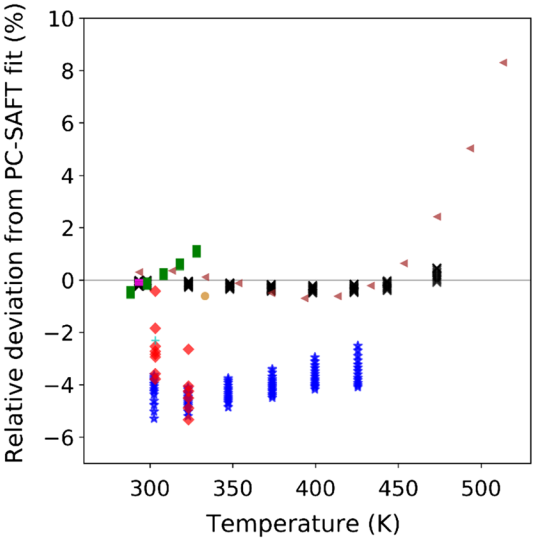

Fig. 2 Comparison of the literature sources that give the density of tetrahydrofuran at elevated pressures. ×This work, —[58], ●[59], ■[60], ◀[61], ◆[62], ★[63], +[64]

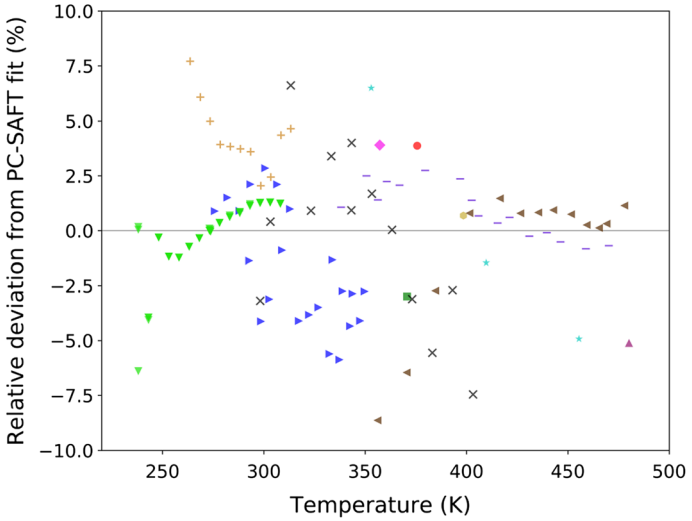

Fig. 3 Comparison of vapor pressure data for gamma-valerolactone from different sources. ×This work, ▼[65], –[66], ■[67], ●[68], ◀[69], ▶[70], ◆[56], ★[71], +[72], ⬢[73], ▲[74]

Table 23 Normal boiling points and enthalpies of vaporization of the bio-compounds

Compound	Normal boiling point[1] (K)		Enthalpy of vaporization[2] at 298.15 K(kJ·mol^{-1})	
	This work	Literature[a]	This work	Literature
2-Methoxy-4-methylphenol	493.9	494.2	64.58	70.9[a]
2-Methylfuran	337.4	337 ± 1	32.11	32.4[b]
2-Pentanone	375.3	375. ± 1	38.26	38.4[a]
2-*sec*-Butylphenol	503.5	500. ± 4	78.38	NA
2,6-Dimethoxyphenol	535.0	536 ± 5	76.69	NA
Cyclopentyl methyl ether	378.6	377.9[c]	37.41	NA
Dihydrolevoglucosenone	499	476[d]	57.65	NA
Furfural	434.1	434.7 ± 0.4	50.57	50.7 ± 0.2
Levoglucosenone	504	NA	61.56	NA
Tetrahydrofuran	339.2	339. ± 1	31.87	32.16[a]
γ-Valerolactone	478.3	480.7	53.83	53.9 ± 0.2[e]

All values were calculated using the PC-SAFT equation of state

NA value is not available at 298.15 K

[a]Ref. [29]

[b]Data from Ref. [29] correlated to obtain value at 298.15 K

[c]Ref. [19] at pressure 99,800 Pa

[d]Ref. [3]

[e]Ref. [70]

[1]At a pressure of 101,325 Pa, standard uncertainty u(normal boiling point this work) = 1.5 K

[2]u(enthalpy of vaporization) = 0.7 kJ·mol^{-1}

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