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

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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].
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

| 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                       |
| 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    | NGFPWHGISWUQOIJ-UHFFFAOYSA-N                   | Sigma-Aldrich                  |
| 2,6-Dimethoxyphenol         | Syringol                     | 91-10-1    | KLIDCXFVHGNNTM-UHFFFAOYSA-N                    | Sigma-Aldrich                  |
| Cyclopentyl methyl ether    | Methoxycyclopentane          | 5614-37-9  | SKTDJAMAYNROS-UHFFFAOYSA-N                     | Sigma-Aldrich                  |
| Dihydrolevoglucosenone      | Cyrene; (5 ~ {R})-6,8-dioxabicyclo[3.2.1]oct-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-Methylhydrofuran-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

\[
P = \frac{m}{W} \cdot \left( \frac{P_{\text{atm}} + \Delta P_{\text{loss}}}{m + \frac{tV}{T_{\text{room}}R}} \right)
\]

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\(^{-1}\), \(P_{\text{atm}}\) is the atmospheric pressure at the place and time the experiment is carried out (Pa), \(T_{\text{room}}\) is room temperature (K), \(R\) is the ideal gas constant, and \(\Delta P_{\text{loss}}\) 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·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      | \(\epsilon/k\) | \(\mu\) | \(n_m\) | \(\kappa^{AB}\) | \(\epsilon^{AB}/k\) | 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          | 3.4a   | 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, \(\sigma\) is the segment diameter (Å), \(\epsilon/k\) is the dispersion energy divided by the Boltzmann constant (K), \(\mu\) is the dipole moment, \(n_m\) is the number of dipole moments, \(\kappa^{AB}\) is the association volume, \(\epsilon^{AB}/k\) 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                 | 968.66                        |
| 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                   |
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.

| 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           |                |                  |                   |

ᵃThe standard uncertainty of the pressure is u(pressure) = 0.0031 MPa (expanded uncertainty u(pressure) = 0.0063 MPa at the 95 % level)
ᵇStandard uncertainty of temperature u(temperature) = 0.1 K (expanded uncertainty u(temperature) = 0.2 K at the 95 % level)
ᶜStandard uncertainty of the density is 0.66 kg·m⁻³ (expanded uncertainty of 1.3 kg·m⁻³ at the 95 % level)
Table 6  Compressed liquid density of 2-Methylfuran

| Pressure (MPa)\(^a\) | Density (kg m\(^{-3}\))\(^c\) | Temperature (K)\(^b\) | Density (kg m\(^{-3}\))\(^c\) | Temperature (K)\(^b\) |
|----------------------|-----------------------------|----------------------|-----------------------------|----------------------|
| 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    293.15     914.86     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     10.01     398.16     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 |
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 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)
Table 7  Compressed liquid density of 2-pentanone

| 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                 | 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                 | 805.65                        | 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                        |
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, 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 7 (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              | 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               | 448.16              | 640.12              |
| 3.948               | 348.15              | 756.24              | 1.101               | 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 \(u(\text{pressure}) = 0.0031\) MPa (expanded uncertainty \(u(\text{pressure}) = 0.0063\) MPa at the 95 % level)

\(^b\)Standard uncertainty of temperature \(u(\text{temperature}) = 0.1\) K (expanded uncertainty \(u(\text{temperature}) = 0.2\) K at the 95 % level)

\(^c\)Standard uncertainty of the density is 0.21 kg·m\(^{-3}\) (expanded uncertainty of 0.41 kg·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·m$^{-3}$)$^c$ | Pressure (MPa)$^a$ | Temperature (K)$^b$ | Density (kg·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              | 866.8                   | 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                    |
| 0.988             | 293.15              | 863.96                    | 6.916             | 398.15              | 766.08                    |
| 11.853            | 293.15              | 872.11                    | 8.890             | 398.15              | 769.16                    |
| 10.886            | 293.15              | 871.40                    | 9.876             | 398.15              | 770.62                    |
| 0.513             | 323.16              | 834.09                    | 7.943             | 423.15              | 741.38                    |
| 0.988             | 323.15              | 833.70                    | 6.959             | 423.15              | 739.49                    |
| 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             | 423.15              | 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 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·m⁻³), but 6 of the 19 sources give a higher density of about 809 kg·m⁻³. So many of the values actually lie more than 1 kg·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

| Pressure (MPa) | Temperature (K) | Density (kg·m⁻³) | Pressure (MPa) | Temperature (K) | Density (kg·m⁻³) |
|---------------|----------------|-----------------|---------------|----------------|-----------------|
| 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          |

*The standard uncertainty of the pressure is \( u(\text{pressure}) = 0.0031 \text{ MPa} \) (expanded uncertainty \( u(\text{pressure} = 0.0063 \text{ MPa} \) at the 95 % level)

bStandard uncertainty of temperature \( u(\text{temperature}) = 0.1 \text{ K} \) (expanded uncertainty \( u(\text{temperature}) = 0.2 \text{ K} \) at the 95 % level)

cStandard uncertainty of the density is 0.10 kg·m⁻³ (expanded uncertainty of 0.20 kg·m⁻³ at the 95 % level)
Table 11: Compressed liquid density of dihydrolevoglucosenone

| Pressure (MPa)$^a$ | Temperature (K)$^b$ | Density (kg·m$^{-3}$)$^c$ | Pressure (MPa)$^a$ | Temperature (K)$^b$ | Density (kg·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             | 373.15              | 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·m$^{-3}$ (expanded uncertainty of 0.51 kg·m$^{-3}$ at the 95 % level)
Table 12  Compressed liquid density of furfural

| Pressure (MPa)\(^a\) | Temperature (K)\(^b\) | Density (kg·m\(^{-3}\))\(^c\) | Pressure (MPa)\(^a\) | Temperature (K)\(^b\) | Density (kg·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          | 12.832                | 373.15                | 1084.37          |
| 10.865                | 293.15                | 1166.40          | 0.092                 | 398.16                | 1044.93          |
| 11.851                | 293.15                | 1167.00          | 0.092                 | 398.15                | 1044.54          |
| 0.988                 | 298.14                | 1154.82          | 0.987                 | 398.15                | 1045.45          |
| 0.993                 | 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          |
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 dihydrolevoglucone and levoglucone 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 dihydrolevoglucone 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 dihydrolevoglucone 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 levoglucone to

| Pressure (MPa)a | Temperature (K)b | Density (kg·m⁻³)c | Pressure (MPa)a | Temperature (K)b | Density (kg·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            |
| 0.807          | 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            |
| 0.901          | 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·m⁻³ (expanded uncertainty of 0.47 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.

| Pressure (MPa) | Temperature (K) | Density (kg m⁻³) |
|---------------|----------------|------------------|
| 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           |

Table 13 Liquid density of levoglucosenone

- The standard uncertainty of the pressure is $u(\text{pressure}) = 0.0031$ MPa (expanded uncertainty $u(\text{pressure}) = 0.0063$ MPa at the 95% level).
- Standard uncertainty of temperature $u(\text{temperature}) = 0.1$ K (expanded uncertainty $u(\text{temperature}) = 0.2$ K at the 95% level).
- Standard uncertainty of the density is 1.7 kg·m⁻³ (expanded uncertainty of 3.4 kg·m⁻³ at the 95% level).
Table 14 Compressed liquid density of tetrahydrofuran

| Pressure (MPa) | Temperature (K) | Density (kg·m⁻³) | Pressure (MPa) | Temperature (K) | Density (kg·m⁻³) |
|---------------|----------------|------------------|---------------|----------------|------------------|
| 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         | 373.15         | 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           |
The standard uncertainty of the pressure is $u(\text{pressure}) = 0.0031 \text{ MPa}$ (expanded uncertainty $u(\text{pressure}) = 0.0063 \text{ MPa}$ at the 95 % level)

Standard uncertainty of temperature $u(\text{temperature}) = 0.1 \text{ K}$ (expanded uncertainty $u(\text{temperature}) = 0.2 \text{ K}$ at the 95 % level)

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

| Pressure (MPa)$^a$ | Temperature (K)$^b$ | Density (kg·m$^{-3}$)$^c$ | Pressure (MPa)$^a$ | Temperature (K)$^b$ | Density (kg·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 $u(\text{pressure}) = 0.0031 \text{ MPa}$ (expanded uncertainty $u(\text{pressure}) = 0.0063 \text{ MPa}$ at the 95 % level)

$^b$Standard uncertainty of temperature $u(\text{temperature}) = 0.1 \text{ K}$ (expanded uncertainty $u(\text{temperature}) = 0.2 \text{ K}$ at the 95 % level)

$^c$Standard uncertainty of the density is $0.1 \text{ kg} \cdot \text{m}^{-3}$ (expanded uncertainty of $0.2 \text{ kg} \cdot \text{m}^{-3}$ 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 $u(T) = 0.04 \text{ K}$
Table 16  Vapor pressure of liquid 2-sec-butylphenol

| Temperature K &deg; | 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                                                      |

&superscript;Standard uncertainty of the temperature u(T) = 0.04 K

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

| Temperature K &deg; | 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                                                       |

&superscript;Standard uncertainty of the temperature u(T) = 0.04 K
**Table 18** Vapor pressure of liquid Dihydrolevoglucosenone (cyrene)

| Temperature K | 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                                                     |

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

**Table 19** Vapor pressure of liquid Levoglucosenone

| Temperature (K) | 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                                                     |

*aStandard 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                                                    |

aStandard 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<sup>a</sup> | Refractive index<sup>b</sup> |
|--------------------------|-------------------------------|
|                          | Dihydrolevoglucosenone (cyrene) | γ-Valerolactone (creosol) | 2-Methoxy-4-methylphenol (creosol) | 2-sec-Butylphenol | Levoglucosenone | 2,6-Dimethoxyphenol (syringol) | Tetrahydrofuran | 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             |                  |                                  | 1.4073          | 1.3903       | 1.4332       |
| 303.15                   | 1.4691                        | 1.4292                     | 1.5323                              | 1.5171             | 1.5022           |                                  | 1.4073          | 1.3903       | 1.4332       |
| 308.15                   | 1.4671                        | 1.4272                     | 1.5299                              | 1.5146             |                  |                                  | 1.4073          | 1.3903       | 1.4332       |
| 313.15                   | 1.4651                        | 1.4252                     | 1.5274                              | 1.5113             | 1.4980           |                                  | 1.4073          | 1.3903       | 1.4332       |
| 318.15                   | 1.4631                        | 1.4231                     | 1.525                               | 1.5086             |                  |                                  | 1.4073          | 1.3903       | 1.4332       |
| 323.15                   | 1.4611                        | 1.4211                     | 1.5225                              | 1.5062             | 1.4938           |                                  | 1.4073          | 1.3903       | 1.4332       |
| 328.15                   | 1.4592                        | 1.4191                     | 1.5200                              | 1.5039             | 1.5365           |                                  | 1.4073          | 1.3903       | 1.4332       |
| 333.15                   | 1.4571                        | 1.4170                     | 1.5176                              | 1.5018             | 1.4896           | 1.5344               | 1.4073          | 1.3903       | 1.4332       |
| 338.15                   |                              |                            | 1.5151                              | 1.5000             | 1.5320           | 1.5365               | 1.4073          | 1.3903       | 1.4332       |
| 343.15                   |                              |                            | 1.5126                              | 1.4980             | 1.4854           | 1.5296               | 1.4073          | 1.3903       | 1.4332       |

Standard uncertainty of the pressure is 0.01 MPa

<sup>a</sup>Standard uncertainty of the temperature is 0.03 K

<sup>b</sup>Standard uncertainty of liquid refractive index: \( u(\text{refractive index}) = 0.0034 \), (expanded uncertainty of 0.0078 at the 95 % level)
Table 22  Comparison of experimental density values from this study with literature values

| Compound                  | Density at 293.15 K (kg·m⁻³) | References                        |
|---------------------------|------------------------------|-----------------------------------|
| This work                 | Literature"                  |
| 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 ± 0.22b               | 980.4b [101]                      |
| 2,6-Dimethoxyphenol       | 1158.57 ± 0.6c               | –                                 |
| Cyclopentyl methyl ether  | 862.95 ± 0.2                 | 862.80 [102]                      |
|                           |                              | 860.43 [103]                      |
| Dihydrolevoglucosenone    | 1250.75 ± 0.51               | 1250 [3]                          |
|                           |                              | 1251.7 [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 \(u(\text{normal boiling point this work}) = 1.5 \text{ K}\)

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