Supporting Information for:

Evaluation of association schemes in the CPA and PC-SAFT equations in modelling VLE of organic acids + water systems

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# Thermodynamic models

## CPA

The CPA EoS in terms of the residual Helmholtz free energy () is ([Kontogeorgis and Folas 2010](#_ENREF_9)):

|  |  |
| --- | --- |
|  | (S1) |

Where is the residual free energy for the physical interactions calculated from the Soave-Redlich-Kwong (SRK) EoS ([Michelsen and Mollerup 2007](#_ENREF_14)):

|  |  |
| --- | --- |
|  | (S2) |

and are computed from van der Waals one-fluid mixing rules according to:

|  |  |
| --- | --- |
|  | (S3) |

|  |  |
| --- | --- |
|  | (S4) |

with the following classical combining rules:

|  |  |
| --- | --- |
|  | (S5) |

|  |  |
| --- | --- |
|  | (S6) |

where and are binary interaction parameters. For the case in which , as it is often assumed, Eq. (S4) reduces to:

|  |  |
| --- | --- |
|  | (S7) |

The energy parameter is computed from:

|  |  |
| --- | --- |
|  | (S8) |

where and , as well as (in Eq. (S7)) are characteristic parameters for a given compound.

The association term is similar as the one use in PC-SAFT (defined in the next section), but in this case the association strength is computed from:

|  |  |
| --- | --- |
|  | (S9) |

where the simplified radial distribution function ([Kontogeorgis et al. 1999](#_ENREF_12); [Kontogeorgis et al. 2006a](#_ENREF_10)) is:

|  |  |
| --- | --- |
|  | (S10) |

and

|  |  |
| --- | --- |
|  | (S11) |

and are the association energy and association volume parameters respectively. Thus for an associating molecule, five pure component parameters are needed: , , , and , which are usually obtained from fitting vapour pressures and liquid density data.

Several combining rules have been proposed for the association strength in the CPA framework, but the so called Elliot combining rule (ECR) and the CR1 have been the most successful ([Folas 2006](#_ENREF_5); [Kontogeorgis et al. 2006a](#_ENREF_10), [2006b](#_ENREF_11)):

CR1:

|  |  |
| --- | --- |
|  | (S12) |

|  |  |
| --- | --- |
|  | (S13) |

ECR:

|  |  |
| --- | --- |
|  | (S14) |

|  |  |
| --- | --- |
|  | (S15) |

## PC-SAFT / PCP-SAFT

The PC-SAFT EoS expressed in terms of is ([Gross and Sadowski 2001](#_ENREF_6), [2002](#_ENREF_7)):

|  |  |
| --- | --- |
|  | (S16) |

Where , , and are the hard-chain formation, dispersion and association contributions respectively, to the Helmholtz free energy of the system.

When the polar term is included in the expansion in equation (S16), the equation is termed PC-polar SAFT, i.e. ([Gross and Vrabec 2006](#_ENREF_8)):

|  |  |
| --- | --- |
|  | (S17) |

### Hard-chain term

The Helmholtz energy due to chain formation for mixtures is given as:

|  |  |
| --- | --- |
|  | (S18) |

where is the number of moles of compound . is the mean segment number in the mixture, computed from:

|  |  |
| --- | --- |
|  | (S19) |

The radial distribution function for the hard-sphere () fluid is given by:

|  |  |
| --- | --- |
|  | (S20) |

And the Helmholtz free energy due to the hard-sphere segments by:

|  |  |
| --- | --- |
|  | (S21) |

with

|  |  |
| --- | --- |
|  | (S22) |

in Eq. (S22) is defined as the total number density of molecules. The temperature-dependent segment diameter is obtained from:

|  |  |
| --- | --- |
|  | (S23) |

### Dispersion term

The dispersion term is:

|  |  |
| --- | --- |
|  | (S24) |

with:

|  |  |
| --- | --- |
|  | (S25) |

and the following power series function of reduced density, , and the mean segment number:

|  |  |
| --- | --- |
|  | (S26) |

|  |  |
| --- | --- |
|  | (S27) |

The coefficients and are functions of according to:

|  |  |
| --- | --- |
|  | (S28) |

|  |  |
| --- | --- |
|  | (S29) |

Values for the coefficients in Eqs. (S28) and (S29) are reported in the original publication ([Gross and Sadowski 2001](#_ENREF_6)).

For mixtures, conventional Berthelot-Lorenz combining rules are employed introducing one adjustable interaction parameter, , to correct for the mixture dispersion energy:

|  |  |
| --- | --- |
|  | (S30) |

|  |  |
| --- | --- |
|  | (S31) |

Three pure component parameters are thus needed to characterize a non-associating molecule: the number of segments per chain (), the temperature- independent segment diameter () and the depth of the potential well (); usually obtained from fitting vapour pressures and saturated liquid density data.

### Association term

The association contributions are computed from:

|  |  |
| --- | --- |
|  | (S32) |

where is the fraction of molecules of component that are not bonded at the association site , given by the following implicit equation:

|  |  |
| --- | --- |
|  | (S33) |

The term can be seen as a strength of association computed from:

|  |  |
| --- | --- |
|  | (S34) |

The radial distribution function for the segments, , in Eq. (S34) is approximated by that of the hard-sphere fluid expression, i.e.:

|  |  |
| --- | --- |
|  | (S35) |

The association term introduces two additional pure component parameters: the association volume, , and the association energy, , between site and site of component , also treated as adjustable parameters. Combining rules of Wolbach and Sandler are used for mixtures ([Gross and Sadowski 2002](#_ENREF_7)).

|  |  |
| --- | --- |
|  | (S36) |

|  |  |
| --- | --- |
|  | (S37) |

### Polar term

The dipolar contributions in PCP-SAFT are given by ([Gross and Vrabec 2006](#_ENREF_8)):

|  |  |
| --- | --- |
|  | (S38) |

where and are second and third-order perturbation terms:

|  |  |
| --- | --- |
|  | (S39) |

|  |  |
| --- | --- |
|  | (S40) |

where is the number of dipolar segments in a molecule . and are power series of the reduced density, according to:

|  |  |
| --- | --- |
|  | (S41) |

|  |  |
| --- | --- |
|  | (S42) |

The coefficients , and depend on the chain length as:

|  |  |
| --- | --- |
|  | (S43) |

|  |  |
| --- | --- |
|  | (S44) |

|  |  |
| --- | --- |
|  | (S45) |

with

|  |  |
| --- | --- |
|  | (S46) |

|  |  |
| --- | --- |
|  | (S47) |

The values for the constants in Eqs. (S43) – (S45) are reported in the original publication ([Gross and Vrabec 2006](#_ENREF_8)).

# Experimental data

Table S1. Sources of experimental data used in the fitting procedure and evaluation.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| formic acid | |  | propanoic acid | |
| *T* / K | Reference |  | *T* / K | Reference |
| 303.1 | [Udovenko and Aleksandrova (1960)](#_ENREF_23) |  | 303.2 | [Wright and Akhtar (1970)](#_ENREF_25) |
| 318.1 | [Udovenko and Aleksandrova (1960)](#_ENREF_23) |  | 313.1 | [Brazauskiene et al. (1965)](#_ENREF_3) |
| 323.1 | [Campbell and Campbell (1934)](#_ENREF_4) |  | 343.2 | [Miyamoto et al. (2001)](#_ENREF_15) |
| 328.1 | [Tunik and Zharov (1980)](#_ENREF_22) |  | 373.1 | [Rafflenbeul and Hartmann (1978)](#_ENREF_16) |
| 333.1 | [Udovenko and Aleksandrova (1960)](#_ENREF_23) |  | 423.2 | [Román-Ramírez et al. (2015)](#_ENREF_18) |
| 353.1 | [Vrevskii and Glagoleva (1927)](#_ENREF_24) |  | 453.2 | [Román-Ramírez et al. (2015)](#_ENREF_18) |
| 388.2 | [Sommer et al. (2016)](#_ENREF_21) |  | 483.2 | [Román-Ramírez et al. (2015)](#_ENREF_18) |
| 398.2 | [Sommer et al. (2016)](#_ENREF_21) |  |  |  |
| acetic acid |  |  | butanoic acid | |
| *T* / K | Reference |  | *T* / K | Reference |
| 293.2 | [Lazeeva and Markuzin (1973)](#_ENREF_13) |  | 303.2 | [Wright and Akhtar (1970)](#_ENREF_25) |
| 303.2 | [Wright and Akhtar (1970)](#_ENREF_25) |  |  |  |
| 313.2 | [Lazeeva and Markuzin (1973)](#_ENREF_13) |  | *P* / bar | Reference |
| 343.2 | [Miyamoto et al. (2001)](#_ENREF_15) |  | 0.1333 | [Rivenq (1962)](#_ENREF_17) |
| 363.0 | [Arich and Tagliavini (1958)](#_ENREF_2) |  | 0.5333 | [Rivenq (1962)](#_ENREF_17) |
| 373.1 | [Achary and Narasingrao (1947)](#_ENREF_1) |  | 1.0132 | [Rivenq (1962)](#_ENREF_17) |
| 412.6 | [Román-Ramírez and Leeke (2016)](#_ENREF_19) |  |  |  |
| 443.2 | [Román-Ramírez and Leeke (2016)](#_ENREF_19) |  |  |  |
| 483.2 | [Román-Ramírez and Leeke (2016)](#_ENREF_19) |  |  |  |
|  |  |  |  |  |

# Calculated deviations and binary interaction parameters

Table S2. Deviations (, and ) for predictions () with the EoS studied.a,b

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-CR1 |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 44.81 | 0.13 | 15.27 | 0.09 | 43.38 | 0.12 | 86.68 | 0.18 | 105.77 | 0.11 | 61.62 | 0.13 |
| 318.1 | 37.00 | 0.09 | 13.02 | 0.09 | 40.84 | 0.09 | 70.53 | 0.12 | 86.85 | 0.06 | 52.91 | 0.09 |
| 323.1 | 31.44 | 0.09 | 12.58 | 0.12 | 33.78 | 0.09 | 61.02 | 0.13 | 67.27 | 0.07 | 44.97 | 0.09 |
| 328.1 | 28.69 | 0.06 | 10.07 | 0.11 | 31.71 | 0.06 | 57.33 | 0.10 | 58.29 | 0.05 | 42.17 | 0.06 |
| 333.1 | 29.25 | 0.05 | 9.65 | 0.09 | 33.62 | 0.05 | 56.69 | 0.08 | 68.61 | 0.05 | 43.25 | 0.06 |
| 353.1 | 28.18 | 0.03 | 7.42 | 0.08 | 36.92 | 0.02 | 53.60 | 0.03 | 73.02 | 0.07 | 43.32 | 0.01 |
| 388.2 | 17.89 | 0.07 | 4.00 | 0.02 | 28.29 | 0.10 | 34.90 | 0.11 | 46.54 | 0.11 | 28.79 | 0.10 |
| 398.2 | 15.65 | 0.06 | 2.86 | 0.02 | 26.58 | 0.10 | 31.11 | 0.11 | 40.19 | 0.11 | 25.92 | 0.09 |
| Average | 29.11 | 0.07 | 9.36 | 0.08 | 34.39 | 0.08 | 56.48 | 0.11 | 68.32 | 0.08 | 42.87 | 0.08 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 74.00 | 0.21 | 24.34 | 0.10 | 42.35 | 0.15 | 75.52 | 0.23 | 67.42 | 0.22 | 31.74 | 0.13 |
| 303.2 | 91.54 | 0.23 | 35.46 | 0.11 | 58.80 | 0.17 | 92.23 | 0.24 | 82.71 | 0.22 | 45.12 | 0.14 |
| 313.2 | 49.93 | 0.17 | 17.38 | 0.09 | 35.41 | 0.14 | 56.51 | 0.21 | 48.11 | 0.20 | 25.25 | 0.13 |
| 343.2 | 34.26 | 0.16 | 13.98 | 0.07 | 24.99 | 0.11 | 39.36 | 0.18 | 30.39 | 0.15 | 17.09 | 0.09 |
| 363.0 | 29.31 | 0.11 | 12.56 | 0.06 | 28.96 | 0.10 | 35.20 | 0.14 | 28.95 | 0.12 | 18.49 | 0.09 |
| 373.1 | 28.75 | 0.06 | 9.88 | 0.05 | 33.47 | 0.07 | 35.42 | 0.09 | 28.92 | 0.09 | 21.17 | 0.07 |
| 412.6 | 15.22 |  | 8.45 |  | 20.51 |  | 17.58 |  | 14.21 |  | 10.74 |  |
| 443.2 | 10.91 |  | 7.54 |  | 17.11 |  | 11.53 |  | 9.94 |  | 8.14 |  |
| 483.2 | 8.22 |  | 5.63 |  | 16.73 |  | 9.08 |  | 7.57 |  | 7.41 |  |
| Average | 38.01 | 0.15 | 15.02 | 0.08 | 30.93 | 0.12 | 41.38 | 0.18 | 35.36 | 0.17 | 20.57 | 0.11 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 35.80 | 0.14 | 60.87 | 0.12 | 75.40 | 0.11 | 128.62 | 0.18 | 130.38 | 0.17 | 49.97 | 0.07 |
| 313.1 | 42.43 | 0.18 | 46.65 | 0.22 | 33.53 | 0.14 | 95.29 | 0.31 | 112.51 | 0.31 | 15.91 | 0.07 |
| 343.2 | 23.06 | 0.10 | 20.20 | 0.12 | 26.23 | 0.11 | 39.43 | 0.16 | 31.24 | 0.15 | 13.23 | 0.06 |
| 373.1 | 17.29 | 0.06 | 15.86 | 0.06 | 24.10 | 0.08 | 26.05 | 0.11 | 28.11 | 0.11 | 9.05 | 0.05 |
| 423.2 | 18.87 | 0.09 | 15.43 | 0.09 | 21.44 | 0.11 | 16.39 | 0.07 | 11.11 | 0.07 | 10.91 | 0.07 |
| 453.2 | 15.23 | 0.12 | 14.34 | 0.12 | 18.05 | 0.13 | 12.35 | 0.10 | 13.08 | 0.10 | 10.18 | 0.10 |
| 483.2 | 11.73 | 0.17 | 12.53 | 0.17 | 14.67 | 0.17 | 9.13 | 0.15 | 10.27 | 0.15 | 8.29 | 0.15 |
| Average | 23.49 | 0.12 | 26.55 | 0.13 | 30.49 | 0.12 | 46.75 | 0.15 | 48.10 | 0.15 | 16.79 | 0.08 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 86.12 | 0.13 | 51.95 | 0.09 | 70.63 | 0.10 | 106.84 | 0.15 | 73.91 | 0.17 | 44.86 | 0.08 |
| Average | 86.12 | 0.13 | 51.95 | 0.09 | 70.63 | 0.10 | 106.84 | 0.15 | 73.91 | 0.17 | 44.86 | 0.08 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 9.17 | 0.16 | 36.36 | 0.14 | 6.39 | 0.09 | 11.05 | 0.18 | 26.49 | 0.40 | 3.67 | 0.06 |
| 0.5333 | 8.10 | 0.11 | 23.14 | 0.12 | 6.80 | 0.07 | 8.50 | 0.12 | 28.40 | 0.13 | 3.76 | 0.05 |
| 1.0132 | 7.06 | 0.10 | 16.30 | 0.11 | 6.35 | 0.07 | 7.15 | 0.10 | 20.04 | 0.10 | 3.35 | 0.04 |
| Average | 8.11 | 0.12 | 25.27 | 0.12 | 6.52 | 0.08 | 8.90 | 0.13 | 24.97 | 0.21 | 3.59 | 0.05 |
| Overall average | 33.02 | 0.11 | 17.92 | 0.10 | 33.50 | 0.11 | 50.34 | 0.14 | 51.01 | 0.13 | 27.62 | 0.09 |

Table S2. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-ECR |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 47.86 | 0.14 | 16.41 | 0.09 | 47.42 | 0.13 | 92.80 | 0.18 | 109.21 | 0.12 | 67.85 | 0.14 |
| 318.1 | 39.43 | 0.09 | 14.72 | 0.09 | 42.98 | 0.10 | 75.39 | 0.13 | 89.52 | 0.07 | 58.34 | 0.10 |
| 323.1 | 33.38 | 0.10 | 13.52 | 0.11 | 36.55 | 0.09 | 65.49 | 0.14 | 69.68 | 0.08 | 49.62 | 0.10 |
| 328.1 | 30.59 | 0.07 | 11.32 | 0.11 | 34.54 | 0.07 | 61.71 | 0.11 | 60.63 | 0.06 | 46.78 | 0.07 |
| 333.1 | 31.23 | 0.05 | 10.96 | 0.09 | 36.70 | 0.06 | 60.82 | 0.09 | 70.83 | 0.05 | 48.02 | 0.07 |
| 353.1 | 30.41 | 0.02 | 8.99 | 0.07 | 39.97 | 0.01 | 57.53 | 0.04 | 75.43 | 0.07 | 48.48 | 0.02 |
| 388.2 | 19.35 | 0.07 | 5.31 | 0.03 | 30.66 | 0.11 | 37.95 | 0.12 | 48.18 | 0.12 | 32.79 | 0.11 |
| 398.2 | 17.03 | 0.06 | 4.12 | 0.02 | 28.83 | 0.10 | 33.98 | 0.12 | 41.74 | 0.11 | 29.74 | 0.10 |
| Average | 31.16 | 0.08 | 10.67 | 0.08 | 37.21 | 0.08 | 60.71 | 0.12 | 70.65 | 0.09 | 47.70 | 0.09 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 88.99 | 0.23 | 31.53 | 0.11 | 55.55 | 0.18 | 93.57 | 0.26 | 82.81 | 0.26 | 47.87 | 0.18 |
| 303.2 | 87.82 | 0.39 | 44.44 | 0.12 | 72.27 | 0.20 | 112.53 | 0.27 | 98.49 | 0.25 | 62.50 | 0.18 |
| 313.2 | 60.83 | 0.19 | 22.61 | 0.10 | 47.03 | 0.16 | 71.70 | 0.25 | 62.41 | 0.24 | 40.56 | 0.17 |
| 343.2 | 41.26 | 0.18 | 15.96 | 0.07 | 31.35 | 0.13 | 51.11 | 0.22 | 41.83 | 0.20 | 26.82 | 0.13 |
| 363.0 | 35.55 | 0.13 | 15.26 | 0.06 | 36.60 | 0.12 | 45.67 | 0.17 | 38.59 | 0.15 | 29.79 | 0.12 |
| 373.1 | 35.42 | 0.07 | 15.54 | 0.04 | 42.33 | 0.09 | 46.05 | 0.11 | 39.20 | 0.10 | 34.33 | 0.10 |
| 412.6 | 17.44 |  | 9.17 |  | 24.21 |  | 23.90 |  | 19.46 |  | 18.31 |  |
| 443.2 | 12.00 |  | 7.30 |  | 19.61 |  | 16.59 |  | 12.99 |  | 13.72 |  |
| 483.2 | 9.37 |  | 5.57 |  | 19.66 |  | 13.43 |  | 10.48 |  | 13.25 |  |
| Average | 43.19 | 0.20 | 18.59 | 0.09 | 38.74 | 0.15 | 52.73 | 0.21 | 45.14 | 0.20 | 31.91 | 0.14 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 57.75 | 0.18 | 84.51 | 0.13 | 102.55 | 0.15 | 176.96 | 0.23 | 159.27 | 0.22 | 83.96 | 0.11 |
| 313.1 | 35.68 | 0.12 | 58.46 | 0.25 | 46.45 | 0.18 | 71.69 | 0.37 | 62.78 | 0.35 | 30.51 | 0.11 |
| 343.2 | 24.27 | 0.12 | 25.55 | 0.12 | 26.85 | 0.11 | 58.20 | 0.22 | 49.46 | 0.21 | 15.77 | 0.09 |
| 373.1 | 22.96 | 0.06 | 17.14 | 0.07 | 33.16 | 0.10 | 43.01 | 0.15 | 37.69 | 0.13 | 21.84 | 0.09 |
| 423.2 | 19.83 | 0.09 | 14.75 | 0.08 | 21.96 | 0.10 | 20.69 | 0.07 | 19.26 | 0.07 | 12.74 | 0.06 |
| 453.2 | 14.36 | 0.11 | 12.26 | 0.11 | 18.47 | 0.12 | 14.21 | 0.09 | 13.29 | 0.09 | 10.50 | 0.09 |
| 483.2 | 10.27 | 0.16 | 9.55 | 0.16 | 14.93 | 0.16 | 9.41 | 0.14 | 9.07 | 0.14 | 7.62 | 0.14 |
| Average | 26.45 | 0.12 | 31.74 | 0.13 | 37.77 | 0.13 | 56.31 | 0.18 | 50.12 | 0.17 | 26.13 | 0.10 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 115.34 | 0.15 | 71.18 | 0.11 | 105.23 | 0.12 | 159.85 | 0.19 | 88.95 | 0.23 | 89.54 | 0.10 |
| Average | 115.34 | 0.15 | 71.18 | 0.11 | 105.23 | 0.12 | 159.85 | 0.19 | 88.95 | 0.23 | 89.54 | 0.10 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 10.65 | 0.17 | 46.48 | 0.14 | 7.31 | 0.07 | 16.53 | 0.20 | 37.29 | 0.16 | 5.93 | 0.05 |
| 0.5333 | 8.77 | 0.12 | 31.02 | 0.10 | 7.40 | 0.07 | 12.91 | 0.16 | 25.82 | 0.11 | 5.86 | 0.06 |
| 1.0132 | 7.61 | 0.10 | 21.92 | 0.09 | 7.59 | 0.07 | 11.59 | 0.15 | 19.76 | 0.09 | 5.78 | 0.06 |
| Average | 9.01 | 0.13 | 33.14 | 0.11 | 7.43 | 0.07 | 13.67 | 0.17 | 27.62 | 0.12 | 5.86 | 0.06 |
| Overall average | 37.54 | 0.13 | 21.84 | 0.10 | 40.63 | 0.12 | 60.57 | 0.17 | 56.45 | 0.15 | 37.65 | 0.11 |

Table S2. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PC-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 9.26 | 0.11 | 17.45 | 0.17 | 9.37 | 0.12 | 55.05 | 0.11 | 44.54 | 0.09 | 47.69 | 0.11 | 25.73 | 0.09 |
| 318.1 | 7.91 | 0.11 | 16.10 | 0.16 | 8.81 | 0.12 | 45.61 | 0.08 | 36.48 | 0.07 | 40.73 | 0.08 | 23.46 | 0.09 |
| 323.1 | 8.00 | 0.12 | 12.48 | 0.18 | 9.08 | 0.13 | 38.20 | 0.08 | 30.36 | 0.07 | 33.84 | 0.07 | 20.37 | 0.10 |
| 328.1 | 5.92 | 0.13 | 11.67 | 0.18 | 6.80 | 0.12 | 35.21 | 0.05 | 27.47 | 0.05 | 31.17 | 0.06 | 18.48 | 0.09 |
| 333.1 | 4.89 | 0.10 | 14.80 | 0.16 | 6.16 | 0.10 | 35.73 | 0.05 | 27.70 | 0.04 | 32.21 | 0.05 | 18.71 | 0.08 |
| 353.1 | 2.66 | 0.09 | 18.18 | 0.15 | 6.07 | 0.09 | 34.51 | 0.02 | 25.95 | 0.04 | 32.59 | 0.03 | 18.73 | 0.08 |
| 388.2 | 1.38 | 0.01 | 16.44 | 0.04 | 3.66 | 0.03 | 20.75 | 0.08 | 13.92 | 0.06 | 19.78 | 0.08 | 9.72 | 0.03 |
| 398.2 | 1.92 | 0.01 | 16.78 | 0.04 | 3.06 | 0.03 | 18.05 | 0.07 | 11.49 | 0.05 | 17.36 | 0.07 | 7.64 | 0.03 |
| Average | 5.24 | 0.09 | 15.49 | 0.14 | 6.63 | 0.09 | 35.39 | 0.07 | 27.24 | 0.06 | 31.92 | 0.07 | 17.86 | 0.07 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 12.83 | 0.04 | 34.69 | 0.14 | 12.68 | 0.04 | 20.66 | 0.09 | 12.73 | 0.07 | 15.64 | 0.08 | 23.45 | 0.13 |
| 303.2 | 4.63 | 0.03 | 28.44 | 0.14 | 5.90 | 0.04 | 31.07 | 0.10 | 22.16 | 0.07 | 26.59 | 0.08 | 36.25 | 0.13 |
| 313.2 | 15.15 | 0.04 | 34.53 | 0.12 | 12.77 | 0.04 | 13.34 | 0.09 | 7.10 | 0.07 | 11.42 | 0.08 | 18.18 | 0.12 |
| 343.2 | 8.81 | 0.03 | 19.63 | 0.08 | 7.23 | 0.03 | 7.42 | 0.05 | 3.85 | 0.03 | 6.55 | 0.05 | 13.11 | 0.06 |
| 363.0 | 13.89 | 0.04 | 29.00 | 0.10 | 10.86 | 0.03 | 6.10 | 0.04 | 1.94 | 0.03 | 6.36 | 0.05 | 12.41 | 0.06 |
| 373.1 | 16.78 | 0.05 | 35.96 | 0.12 | 11.21 | 0.05 | 6.71 | 0.04 | 1.29 | 0.03 | 8.69 | 0.05 | 12.81 | 0.04 |
| 412.6 | 12.60 |  | 23.41 |  | 9.48 |  | 2.17 |  | 4.74 |  | 1.07 |  | 5.03 |  |
| 443.2 | 13.06 |  | 22.11 |  | 9.74 |  | 2.16 |  | 5.74 |  | 1.51 |  | 3.15 |  |
| 483.2 | 12.31 |  | 21.09 |  | 8.05 |  | 2.45 |  | 6.38 |  | 0.80 |  | 3.05 |  |
| Average | 12.23 | 0.04 | 27.65 | 0.11 | 9.77 | 0.04 | 10.23 | 0.07 | 7.33 | 0.05 | 8.74 | 0.06 | 14.16 | 0.09 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 6.79 | 0.04 | 22.23 | 0.10 | 11.33 | 0.02 | 21.07 | 0.02 | 9.46 | 0.03 | 20.48 | 0.02 | 55.65 | 0.08 |
| 313.1 | 14.65 | 0.04 | 28.63 | 0.09 | 10.95 | 0.02 | 7.48 | 0.02 | 11.19 | 0.03 | 6.75 | 0.02 | 18.81 | 0.09 |
| 343.2 | 22.33 | 0.08 | 32.09 | 0.12 | 17.87 | 0.05 | 15.93 | 0.04 | 19.85 | 0.06 | 14.08 | 0.03 | 11.87 | 0.06 |
| 373.1 | 19.87 | 0.04 | 32.09 | 0.09 | 12.10 | 0.02 | 12.74 | 0.02 | 18.60 | 0.03 | 9.23 | 0.02 | 6.82 | 0.04 |
| 423.2 | 21.31 | 0.11 | 30.46 | 0.14 | 15.02 | 0.09 | 16.59 | 0.08 | 20.32 | 0.10 | 13.31 | 0.07 | 9.76 | 0.06 |
| 453.2 | 21.81 | 0.14 | 30.38 | 0.17 | 14.58 | 0.12 | 17.21 | 0.12 | 21.14 | 0.13 | 12.89 | 0.10 | 11.23 | 0.10 |
| 483.2 | 21.67 | 0.18 | 29.58 | 0.20 | 13.60 | 0.16 | 17.10 | 0.16 | 21.19 | 0.17 | 12.08 | 0.15 | 13.30 | 0.14 |
| Average | 18.35 | 0.09 | 29.35 | 0.13 | 13.63 | 0.07 | 15.44 | 0.07 | 17.39 | 0.08 | 12.69 | 0.06 | 18.21 | 0.08 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 7.12 | 0.05 | 26.20 | 0.04 | 13.18 | 0.06 | 8.32 | 0.06 | 5.69 | 0.05 | 11.76 | 0.06 | 51.07 | 0.09 |
| Average | 7.12 | 0.05 | 26.20 | 0.04 | 13.18 | 0.06 | 8.32 | 0.06 | 5.69 | 0.05 | 11.76 | 0.06 | 51.07 | 0.09 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 6.67 | 0.08 | 11.56 | 0.11 | 3.36 | 0.05 | 5.30 | 0.06 | 7.68 | 0.08 | 3.65 | 0.04 | 3.52 | 0.06 |
| 0.5333 | 8.30 | 0.07 | 12.94 | 0.10 | 4.27 | 0.04 | 6.93 | 0.06 | 9.36 | 0.08 | 4.59 | 0.03 | 3.56 | 0.04 |
| 1.0132 | 8.54 | 0.07 | 12.90 | 0.10 | 4.26 | 0.04 | 7.24 | 0.06 | 9.64 | 0.07 | 4.68 | 0.03 | 3.45 | 0.04 |
| Average | 7.84 | 0.07 | 12.47 | 0.10 | 3.96 | 0.04 | 6.49 | 0.06 | 8.89 | 0.08 | 4.31 | 0.03 | 3.51 | 0.05 |
| Overall average | 11.50 | 0.07 | 24.18 | 0.12 | 9.98 | 0.07 | 19.67 | 0.07 | 16.45 | 0.06 | 17.38 | 0.06 | 17.95 | 0.08 |

Table S2. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PCP-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 31.32 | 0.12 | 10.08 | 0.13 | 37.43 | 0.14 | 104.80 | 0.20 | 97.50 | 0.18 | 92.36 | 0.18 | 34.40 | 0.10 |
| 318.1 | 26.35 | 0.10 | 8.58 | 0.13 | 32.19 | 0.11 | 84.14 | 0.14 | 77.74 | 0.13 | 75.73 | 0.13 | 30.63 | 0.09 |
| 323.1 | 21.68 | 0.10 | 7.97 | 0.14 | 26.06 | 0.11 | 71.78 | 0.15 | 65.70 | 0.13 | 63.72 | 0.13 | 25.53 | 0.09 |
| 328.1 | 19.07 | 0.09 | 7.27 | 0.14 | 23.35 | 0.09 | 67.55 | 0.12 | 61.44 | 0.10 | 59.86 | 0.10 | 23.31 | 0.09 |
| 333.1 | 19.55 | 0.08 | 6.19 | 0.12 | 24.73 | 0.08 | 67.08 | 0.10 | 60.76 | 0.09 | 60.59 | 0.09 | 24.35 | 0.07 |
| 353.1 | 19.11 | 0.07 | 3.14 | 0.12 | 25.78 | 0.06 | 63.65 | 0.04 | 56.96 | 0.03 | 58.85 | 0.03 | 25.55 | 0.07 |
| 388.2 | 9.17 | 0.04 | 4.70 | 0.02 | 14.45 | 0.06 | 41.32 | 0.14 | 35.48 | 0.12 | 37.96 | 0.13 | 13.70 | 0.05 |
| 398.2 | 7.19 | 0.04 | 5.52 | 0.02 | 12.35 | 0.06 | 36.99 | 0.13 | 31.37 | 0.11 | 33.99 | 0.12 | 11.37 | 0.05 |
| Average | 19.18 | 0.08 | 6.68 | 0.10 | 24.54 | 0.09 | 67.16 | 0.13 | 60.87 | 0.11 | 60.38 | 0.11 | 23.61 | 0.08 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 21.26 | 0.09 | 5.65 | 0.02 | 30.56 | 0.13 | 71.47 | 0.23 | 61.25 | 0.21 | 69.07 | 0.23 | 37.03 | 0.17 |
| 303.2 | 30.51 | 0.08 | 7.40 | 0.04 | 40.79 | 0.12 | 84.03 | 0.23 | 70.45 | 0.20 | 81.51 | 0.22 | 50.75 | 0.17 |
| 313.2 | 13.37 | 0.06 | 8.65 | 0.03 | 22.77 | 0.10 | 55.23 | 0.21 | 41.70 | 0.18 | 55.29 | 0.21 | 30.30 | 0.16 |
| 343.2 | 4.99 | 0.03 | 6.45 | 0.02 | 10.06 | 0.05 | 30.72 | 0.15 | 23.15 | 0.12 | 30.28 | 0.14 | 19.01 | 0.09 |
| 363.0 | 3.17 | 0.02 | 11.54 | 0.03 | 10.31 | 0.05 | 31.47 | 0.13 | 23.16 | 0.11 | 32.49 | 0.13 | 19.75 | 0.08 |
| 373.1 | 3.82 | 0.03 | 13.53 | 0.05 | 13.83 | 0.05 | 35.17 | 0.10 | 26.02 | 0.09 | 37.45 | 0.11 | 22.47 | 0.07 |
| 412.6 | 3.03 |  | 12.21 |  | 3.19 |  | 15.09 |  | 9.24 |  | 16.42 |  | 8.90 |  |
| 443.2 | 5.64 |  | 13.12 |  | 2.16 |  | 9.56 |  | 5.34 |  | 10.72 |  | 4.13 |  |
| 483.2 | 6.16 |  | 12.95 |  | 1.44 |  | 7.10 |  | 3.24 |  | 8.94 |  | 1.72 |  |
| Average | 10.22 | 0.05 | 10.17 | 0.03 | 15.01 | 0.08 | 37.76 | 0.17 | 29.28 | 0.15 | 38.02 | 0.18 | 21.56 | 0.12 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 61.18 | 0.08 | 25.56 | 0.02 | 96.19 | 0.13 | 100.11 | 0.13 | 80.78 | 0.11 | 114.93 | 0.15 | 89.64 | 0.12 |
| 313.1 | 13.97 | 0.06 | 5.03 | 0.02 | 31.09 | 0.10 | 35.21 | 0.12 | 24.31 | 0.09 | 39.99 | 0.12 | 32.78 | 0.12 |
| 343.2 | 9.19 | 0.04 | 14.11 | 0.04 | 15.47 | 0.08 | 14.71 | 0.09 | 10.65 | 0.06 | 19.77 | 0.11 | 13.56 | 0.07 |
| 373.1 | 5.47 | 0.04 | 10.21 | 0.02 | 20.40 | 0.08 | 17.45 | 0.08 | 10.04 | 0.06 | 25.01 | 0.10 | 15.44 | 0.07 |
| 423.2 | 7.02 | 0.07 | 15.02 | 0.09 | 11.75 | 0.08 | 7.95 | 0.05 | 6.48 | 0.05 | 10.04 | 0.05 | 7.77 | 0.05 |
| 453.2 | 8.91 | 0.11 | 16.10 | 0.12 | 9.34 | 0.11 | 5.78 | 0.08 | 6.59 | 0.09 | 7.55 | 0.08 | 6.24 | 0.08 |
| 483.2 | 10.04 | 0.15 | 16.93 | 0.16 | 7.04 | 0.15 | 3.84 | 0.13 | 7.53 | 0.14 | 4.42 | 0.13 | 6.26 | 0.12 |
| Average | 16.54 | 0.08 | 14.71 | 0.07 | 27.33 | 0.10 | 26.44 | 0.10 | 20.91 | 0.09 | 31.67 | 0.11 | 24.53 | 0.09 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 74.25 | 0.09 | 36.36 | 0.07 | 140.30 | 0.13 | 97.07 | 0.11 | 72.55 | 0.09 | 135.81 | 0.12 | 98.80 | 0.11 |
| Average | 74.25 | 0.09 | 36.36 | 0.07 | 140.30 | 0.13 | 97.07 | 0.11 | 72.55 | 0.09 | 135.81 | 0.12 | 98.80 | 0.11 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 3.88 | 0.04 | 2.04 | 0.04 | 8.68 | 0.07 | 5.39 | 0.04 | 3.75 | 0.04 | 8.33 | 0.07 | 6.03 | 0.06 |
| 0.5333 | 3.05 | 0.03 | 2.53 | 0.03 | 7.68 | 0.07 | 3.89 | 0.04 | 2.67 | 0.03 | 7.30 | 0.07 | 4.47 | 0.04 |
| 1.0132 | 2.29 | 0.03 | 2.76 | 0.03 | 7.19 | 0.07 | 3.09 | 0.03 | 1.88 | 0.03 | 6.61 | 0.06 | 3.52 | 0.04 |
| Average | 3.07 | 0.04 | 2.44 | 0.03 | 7.85 | 0.07 | 4.12 | 0.04 | 2.77 | 0.03 | 7.41 | 0.07 | 4.67 | 0.05 |
| Overall average | 17.42 | 0.07 | 11.37 | 0.07 | 26.52 | 0.09 | 46.37 | 0.13 | 38.78 | 0.11 | 47.31 | 0.13 | 26.14 | 0.10 |
| a Overall average values computed from isothermal data only.  b Values for CPA-CR1 2B-2B taken from ([Román-Ramírez and Leeke 2020](#_ENREF_20)), except isobaric data. | | | | | | | | | | | | | | |

Table S3. Deviations (, and ) for correlations () with the EoS studied.a,b

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-CR1 |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 4.38 | 0.11 | 6.30 | 0.12 | 4.61 | 0.12 | 9.80 | 0.13 | 11.45 | 0.14 | 10.67 | 0.13 |
| 318.1 | 4.39 | 0.11 | 5.14 | 0.12 | 6.13 | 0.11 | 8.73 | 0.12 | 9.93 | 0.14 | 9.30 | 0.13 |
| 323.1 | 5.90 | 0.13 | 6.04 | 0.14 | 5.04 | 0.13 | 9.08 | 0.13 | 7.61 | 0.16 | 8.95 | 0.14 |
| 328.1 | 3.89 | 0.13 | 4.58 | 0.13 | 3.19 | 0.13 | 7.18 | 0.13 | 5.80 | 0.16 | 7.38 | 0.13 |
| 333.1 | 2.93 | 0.10 | 3.72 | 0.11 | 2.12 | 0.10 | 6.04 | 0.11 | 6.12 | 0.13 | 6.34 | 0.11 |
| 353.1 | 1.94 | 0.09 | 2.67 | 0.09 | 2.70 | 0.08 | 4.18 | 0.11 | 5.68 | 0.12 | 4.85 | 0.11 |
| 388.2 | 0.96 | 0.02 | 1.17 | 0.01 | 1.39 | 0.02 | 2.88 | 0.02 | 1.92 | 0.01 | 3.28 | 0.03 |
| 398.2 | 0.84 | 0.02 | 1.15 | 0.01 | 1.19 | 0.02 | 2.83 | 0.02 | 1.74 | 0.01 | 3.08 | 0.02 |
| Average | 3.15 | 0.09 | 3.85 | 0.09 | 3.30 | 0.09 | 6.34 | 0.10 | 6.28 | 0.11 | 6.73 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 7.73 | 0.05 | 9.73 | 0.06 | 5.54 | 0.04 | 4.89 | 0.03 | 7.68 | 0.05 | 3.48 | 0.02 |
| 303.2 | 7.13 | 0.04 | 7.05 | 0.04 | 6.41 | 0.04 | 6.36 | 0.02 | 7.59 | 0.04 | 5.33 | 0.02 |
| 313.2 | 8.15 | 0.05 | 9.73 | 0.06 | 6.57 | 0.05 | 5.79 | 0.03 | 6.58 | 0.05 | 4.30 | 0.03 |
| 343.2 | 5.34 | 0.04 | 6.49 | 0.04 | 4.34 | 0.03 | 3.09 | 0.02 | 6.19 | 0.03 | 2.44 | 0.02 |
| 363.0 | 5.63 | 0.04 | 6.86 | 0.04 | 4.21 | 0.03 | 3.15 | 0.02 | 4.87 | 0.04 | 1.95 | 0.02 |
| 373.1 | 4.52 | 0.03 | 5.64 | 0.04 | 3.22 | 0.04 | 2.13 | 0.02 | 3.00 | 0.04 | 1.20 | 0.03 |
| 412.6 | 4.68 |  | 5.53 |  | 3.73 |  | 2.81 |  | 4.83 |  | 2.12 |  |
| 443.2 | 5.50 |  | 6.33 |  | 4.94 |  | 3.54 |  | 6.25 |  | 2.81 |  |
| 483.2 | 4.02 |  | 4.71 |  | 3.37 |  | 2.46 |  | 3.72 |  | 1.96 |  |
| Average | 5.85 | 0.04 | 6.90 | 0.05 | 4.70 | 0.04 | 3.80 | 0.03 | 5.63 | 0.04 | 2.84 | 0.02 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 15.09 | 0.06 | 12.60 | 0.06 | 13.46 | 0.04 | 10.75 | 0.04 | 23.93 | 0.05 | 11.53 | 0.03 |
| 313.1 | 11.61 | 0.05 | 14.13 | 0.05 | 10.34 | 0.03 | 11.03 | 0.04 | 15.79 | 0.04 | 9.55 | 0.03 |
| 343.2 | 16.33 | 0.08 | 17.46 | 0.09 | 17.02 | 0.07 | 15.10 | 0.06 | 11.84 | 0.06 | 14.81 | 0.05 |
| 373.1 | 11.97 | 0.04 | 13.36 | 0.05 | 8.50 | 0.03 | 9.51 | 0.03 | 8.93 | 0.04 | 7.12 | 0.03 |
| 423.2 | 13.00 | 0.09 | 13.80 | 0.09 | 10.47 | 0.09 | 11.28 | 0.07 | 10.74 | 0.06 | 9.70 | 0.07 |
| 453.2 | 13.20 | 0.12 | 14.18 | 0.12 | 11.56 | 0.13 | 10.95 | 0.10 | 12.31 | 0.10 | 9.84 | 0.10 |
| 483.2 | 11.52 | 0.17 | 12.51 | 0.17 | 10.31 | 0.17 | 9.00 | 0.15 | 10.25 | 0.15 | 8.27 | 0.15 |
| Average | 13.25 | 0.09 | 14.01 | 0.09 | 11.67 | 0.08 | 11.09 | 0.07 | 13.40 | 0.07 | 10.12 | 0.07 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 12.80 | 0.04 | 16.68 | 0.04 | 10.14 | 0.04 | 11.24 | 0.05 | 12.57 | 0.05 | 7.13 | 0.05 |
| Average | 12.80 | 0.04 | 16.68 | 0.04 | 10.14 | 0.04 | 11.24 | 0.05 | 12.57 | 0.05 | 7.13 | 0.05 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 3.89 | 0.06 | 11.11 | 0.11 | 3.12 | 0.06 | 3.27 | 0.05 | 12.70 | 0.11 | 2.39 | 0.05 |
| 0.5333 | 3.55 | 0.04 | 3.65 | 0.04 | 3.24 | 0.05 | 2.90 | 0.04 | 4.36 | 0.05 | 2.54 | 0.03 |
| 1.0132 | 3.91 | 0.05 | 3.99 | 0.03 | 2.94 | 0.04 | 3.20 | 0.05 | 3.12 | 0.03 | 2.55 | 0.03 |
| Average | 3.78 | 0.05 | 6.25 | 0.06 | 3.10 | 0.05 | 3.12 | 0.04 | 6.73 | 0.06 | 2.49 | 0.04 |
| Overall average | 7.34 | 0.07 | 8.30 | 0.08 | 6.42 | 0.07 | 6.95 | 0.07 | 8.29 | 0.07 | 6.30 | 0.07 |

Table S3. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-ECR |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 4.53 | 0.11 | 5.90 | 0.12 | 4.31 | 0.12 | 10.02 | 0.13 | 11.13 | 0.14 | 11.35 | 0.13 |
| 318.1 | 4.35 | 0.11 | 5.38 | 0.12 | 4.81 | 0.11 | 8.96 | 0.12 | 9.58 | 0.14 | 9.94 | 0.13 |
| 323.1 | 5.98 | 0.13 | 6.33 | 0.14 | 5.46 | 0.13 | 9.20 | 0.13 | 7.22 | 0.15 | 9.30 | 0.14 |
| 328.1 | 3.97 | 0.13 | 4.69 | 0.14 | 3.72 | 0.13 | 7.35 | 0.13 | 5.85 | 0.15 | 7.84 | 0.13 |
| 333.1 | 2.94 | 0.11 | 3.62 | 0.11 | 2.68 | 0.11 | 6.25 | 0.11 | 5.91 | 0.13 | 6.92 | 0.12 |
| 353.1 | 1.58 | 0.09 | 1.61 | 0.09 | 1.32 | 0.08 | 4.41 | 0.11 | 5.65 | 0.11 | 5.57 | 0.11 |
| 388.2 | 0.74 | 0.01 | 0.68 | 0.01 | 1.16 | 0.02 | 3.08 | 0.02 | 1.88 | 0.01 | 3.86 | 0.03 |
| 398.2 | 0.72 | 0.01 | 0.62 | 0.01 | 1.12 | 0.02 | 3.01 | 0.02 | 2.10 | 0.01 | 3.56 | 0.03 |
| Average | 3.10 | 0.09 | 3.60 | 0.09 | 3.07 | 0.09 | 6.54 | 0.10 | 6.16 | 0.11 | 7.29 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 5.97 | 0.04 | 7.27 | 0.05 | 5.23 | 0.02 | 3.74 | 0.02 | 6.38 | 0.04 | 2.74 | 0.02 |
| 303.2 | 8.27 | 0.03 | 6.72 | 0.03 | 5.93 | 0.02 | 7.06 | 0.02 | 8.01 | 0.03 | 8.40 | 0.03 |
| 313.2 | 6.34 | 0.04 | 7.49 | 0.04 | 5.49 | 0.03 | 4.54 | 0.03 | 7.22 | 0.04 | 2.78 | 0.02 |
| 343.2 | 4.28 | 0.03 | 5.04 | 0.03 | 2.54 | 0.02 | 2.37 | 0.02 | 5.02 | 0.03 | 1.16 | 0.02 |
| 363.0 | 4.12 | 0.03 | 4.97 | 0.03 | 2.70 | 0.02 | 2.06 | 0.02 | 4.10 | 0.03 | 0.91 | 0.02 |
| 373.1 | 2.71 | 0.03 | 3.49 | 0.03 | 1.21 | 0.03 | 1.13 | 0.02 | 1.56 | 0.03 | 2.27 | 0.03 |
| 412.6 | 3.69 |  | 4.22 |  | 2.35 |  | 2.08 |  | 2.96 |  | 0.95 |  |
| 443.2 | 4.43 |  | 5.04 |  | 3.52 |  | 2.69 |  | 3.66 |  | 1.60 |  |
| 483.2 | 3.09 |  | 3.54 |  | 2.23 |  | 1.70 |  | 2.38 |  | 0.82 |  |
| Average | 4.77 | 0.03 | 5.31 | 0.03 | 3.47 | 0.02 | 3.04 | 0.02 | 4.59 | 0.03 | 2.40 | 0.02 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 13.93 | 0.04 | 14.18 | 0.04 | 17.78 | 0.02 | 13.26 | 0.02 | 16.51 | 0.03 | 16.38 | 0.01 |
| 313.1 | 9.65 | 0.03 | 11.81 | 0.04 | 6.73 | 0.02 | 8.66 | 0.03 | 7.81 | 0.03 | 7.43 | 0.02 |
| 343.2 | 14.14 | 0.06 | 14.67 | 0.07 | 13.20 | 0.05 | 13.14 | 0.05 | 10.94 | 0.04 | 11.60 | 0.02 |
| 373.1 | 7.47 | 0.04 | 9.50 | 0.03 | 4.37 | 0.02 | 6.50 | 0.03 | 5.73 | 0.04 | 2.87 | 0.03 |
| 423.2 | 10.95 | 0.08 | 11.33 | 0.08 | 7.44 | 0.09 | 9.17 | 0.06 | 9.89 | 0.06 | 5.80 | 0.06 |
| 453.2 | 10.91 | 0.12 | 11.27 | 0.11 | 7.98 | 0.12 | 8.77 | 0.09 | 9.49 | 0.09 | 5.75 | 0.10 |
| 483.2 | 8.99 | 0.16 | 9.50 | 0.16 | 6.72 | 0.17 | 6.88 | 0.14 | 7.59 | 0.14 | 4.39 | 0.14 |
| Average | 10.86 | 0.08 | 11.75 | 0.08 | 9.18 | 0.07 | 9.48 | 0.06 | 9.71 | 0.06 | 7.75 | 0.05 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 7.54 | 0.05 | 10.56 | 0.05 | 7.97 | 0.05 | 5.82 | 0.05 | 14.49 | 0.05 | 4.21 | 0.06 |
| Average | 7.54 | 0.05 | 10.56 | 0.05 | 7.97 | 0.05 | 5.82 | 0.05 | 14.49 | 0.05 | 4.21 | 0.06 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 2.57 | 0.04 | 8.11 | 0.09 | 1.43 | 0.03 | 2.15 | 0.04 | 3.16 | 0.08 | 0.87 | 0.02 |
| 0.5333 | 2.51 | 0.03 | 4.35 | 0.05 | 1.52 | 0.02 | 2.00 | 0.03 | 2.00 | 0.04 | 0.82 | 0.01 |
| 1.0132 | 2.64 | 0.04 | 3.01 | 0.04 | 1.27 | 0.02 | 2.07 | 0.03 | 1.71 | 0.03 | 0.62 | 0.01 |
| Average | 2.57 | 0.04 | 5.16 | 0.06 | 1.41 | 0.02 | 2.07 | 0.03 | 2.29 | 0.05 | 0.77 | 0.01 |
| Overall average | 6.05 | 0.07 | 6.78 | 0.07 | 5.12 | 0.06 | 6.08 | 0.06 | 6.92 | 0.07 | 5.54 | 0.06 |

Table S3. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PC-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 5.75 | 0.12 | 7.89 | 0.14 | 7.89 | 0.12 | 10.06 | 0.13 | 8.98 | 0.13 | 11.31 | 0.13 | 9.50 | 0.13 |
| 318.1 | 5.46 | 0.11 | 7.29 | 0.13 | 7.01 | 0.12 | 8.51 | 0.12 | 7.54 | 0.12 | 9.66 | 0.13 | 8.91 | 0.13 |
| 323.1 | 6.16 | 0.13 | 7.00 | 0.14 | 7.18 | 0.13 | 8.35 | 0.13 | 7.53 | 0.13 | 9.02 | 0.14 | 8.74 | 0.14 |
| 328.1 | 4.56 | 0.13 | 6.31 | 0.14 | 5.78 | 0.13 | 6.93 | 0.13 | 6.03 | 0.13 | 7.75 | 0.13 | 7.76 | 0.14 |
| 333.1 | 3.38 | 0.11 | 4.99 | 0.12 | 4.98 | 0.11 | 5.64 | 0.11 | 4.72 | 0.11 | 6.71 | 0.12 | 6.64 | 0.12 |
| 353.1 | 1.44 | 0.10 | 3.55 | 0.11 | 2.68 | 0.10 | 4.27 | 0.11 | 3.30 | 0.10 | 5.36 | 0.11 | 6.23 | 0.12 |
| 388.2 | 1.36 | 0.01 | 2.67 | 0.02 | 2.49 | 0.02 | 2.98 | 0.02 | 2.17 | 0.02 | 3.91 | 0.03 | 3.62 | 0.03 |
| 398.2 | 1.59 | 0.01 | 2.72 | 0.02 | 2.53 | 0.02 | 2.87 | 0.02 | 2.14 | 0.02 | 3.73 | 0.03 | 3.58 | 0.03 |
| Average | 3.71 | 0.09 | 5.30 | 0.10 | 5.07 | 0.09 | 6.20 | 0.10 | 5.30 | 0.10 | 7.18 | 0.10 | 6.87 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 2.96 | 0.02 | 1.16 | 0.01 | 2.81 | 0.03 | 2.64 | 0.02 | 2.50 | 0.03 | 1.65 | 0.02 | 7.45 | 0.03 |
| 303.2 | 9.15 | 0.02 | 10.19 | 0.02 | 10.45 | 0.04 | 8.84 | 0.03 | 8.60 | 0.03 | 9.50 | 0.04 | 4.59 | 0.03 |
| 313.2 | 3.41 | 0.02 | 1.76 | 0.01 | 2.19 | 0.02 | 3.41 | 0.03 | 3.53 | 0.03 | 2.09 | 0.03 | 6.03 | 0.03 |
| 343.2 | 2.06 | 0.01 | 1.29 | 0.00 | 2.12 | 0.02 | 1.90 | 0.01 | 2.18 | 0.02 | 1.25 | 0.02 | 3.03 | 0.02 |
| 363.0 | 1.88 | 0.01 | 0.40 | 0.00 | 2.27 | 0.02 | 1.66 | 0.02 | 1.89 | 0.02 | 1.34 | 0.02 | 2.38 | 0.02 |
| 373.1 | 1.46 | 0.02 | 1.68 | 0.02 | 3.07 | 0.03 | 1.62 | 0.02 | 1.52 | 0.03 | 2.64 | 0.03 | 1.24 | 0.02 |
| 412.6 | 2.08 |  | 1.17 |  | 1.93 |  | 1.68 |  | 2.25 |  | 1.18 |  | 2.81 |  |
| 443.2 | 2.81 |  | 1.93 |  | 2.41 |  | 2.14 |  | 2.77 |  | 1.50 |  | 2.90 |  |
| 483.2 | 1.78 |  | 1.18 |  | 1.54 |  | 1.40 |  | 1.96 |  | 0.97 |  | 2.13 |  |
| Average | 3.07 | 0.02 | 2.31 | 0.01 | 3.20 | 0.03 | 2.81 | 0.02 | 3.02 | 0.03 | 2.46 | 0.03 | 3.62 | 0.03 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 12.97 | 0.03 | 13.95 | 0.03 | 20.33 | 0.02 | 15.24 | 0.02 | 16.56 | 0.02 | 18.16 | 0.02 | 12.50 | 0.02 |
| 313.1 | 9.10 | 0.03 | 9.88 | 0.03 | 5.91 | 0.02 | 7.94 | 0.02 | 8.09 | 0.02 | 7.08 | 0.02 | 8.90 | 0.03 |
| 343.2 | 14.98 | 0.05 | 14.08 | 0.05 | 12.54 | 0.04 | 13.51 | 0.04 | 14.06 | 0.05 | 11.72 | 0.02 | 11.15 | 0.05 |
| 373.1 | 7.41 | 0.02 | 6.95 | 0.03 | 4.13 | 0.03 | 5.70 | 0.03 | 6.21 | 0.03 | 3.34 | 0.03 | 6.72 | 0.03 |
| 423.2 | 9.61 | 0.08 | 9.21 | 0.07 | 6.77 | 0.08 | 8.19 | 0.06 | 8.89 | 0.06 | 5.42 | 0.06 | 10.07 | 0.05 |
| 453.2 | 9.80 | 0.11 | 9.35 | 0.11 | 7.34 | 0.11 | 8.02 | 0.09 | 8.57 | 0.09 | 5.40 | 0.09 | 9.63 | 0.08 |
| 483.2 | 8.27 | 0.16 | 7.85 | 0.15 | 6.29 | 0.16 | 6.38 | 0.14 | 6.75 | 0.14 | 4.27 | 0.14 | 7.62 | 0.12 |
| Average | 10.31 | 0.07 | 10.18 | 0.07 | 9.04 | 0.06 | 9.28 | 0.06 | 9.88 | 0.06 | 7.91 | 0.05 | 9.51 | 0.05 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 6.59 | 0.05 | 8.72 | 0.05 | 7.65 | 0.05 | 4.55 | 0.05 | 5.71 | 0.05 | 4.58 | 0.06 | 6.58 | 0.05 |
| Average | 6.59 | 0.05 | 8.72 | 0.05 | 7.65 | 0.05 | 4.55 | 0.05 | 5.71 | 0.05 | 4.58 | 0.06 | 6.58 | 0.05 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 2.35 | 0.04 | 2.70 | 0.04 | 1.71 | 0.04 | 1.85 | 0.03 | 3.03 | 0.05 | 1.00 | 0.02 | 2.42 | 0.04 |
| 0.5333 | 2.29 | 0.03 | 2.17 | 0.03 | 1.92 | 0.03 | 1.74 | 0.02 | 2.96 | 0.04 | 1.02 | 0.02 | 2.19 | 0.03 |
| 1.0132 | 2.29 | 0.03 | 2.34 | 0.03 | 1.62 | 0.02 | 1.70 | 0.02 | 2.63 | 0.03 | 0.81 | 0.01 | 2.33 | 0.03 |
| Average | 2.31 | 0.03 | 2.40 | 0.03 | 1.75 | 0.03 | 1.77 | 0.03 | 2.87 | 0.04 | 0.95 | 0.02 | 2.31 | 0.03 |
| Overall average | 5.44 | 0.06 | 5.73 | 0.06 | 5.61 | 0.06 | 5.78 | 0.06 | 5.78 | 0.06 | 5.58 | 0.06 | 6.43 | 0.06 |

Table S3. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PCP-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 8.32 | 0.13 | 9.74 | 0.14 | 9.14 | 0.13 | 12.11 | 0.13 | 13.09 | 0.12 | 12.89 | 0.13 | 11.63 | 0.13 |
| 318.1 | 7.34 | 0.12 | 8.21 | 0.14 | 8.00 | 0.13 | 10.30 | 0.13 | 11.00 | 0.12 | 10.99 | 0.13 | 10.89 | 0.13 |
| 323.1 | 7.69 | 0.13 | 8.01 | 0.14 | 7.48 | 0.14 | 9.40 | 0.14 | 10.33 | 0.13 | 9.74 | 0.14 | 9.71 | 0.14 |
| 328.1 | 6.13 | 0.14 | 7.11 | 0.15 | 6.82 | 0.14 | 8.22 | 0.14 | 8.12 | 0.13 | 8.83 | 0.13 | 9.01 | 0.13 |
| 333.1 | 5.20 | 0.11 | 6.05 | 0.13 | 5.89 | 0.12 | 7.19 | 0.12 | 6.96 | 0.11 | 7.80 | 0.12 | 8.32 | 0.12 |
| 353.1 | 3.00 | 0.10 | 3.43 | 0.11 | 2.98 | 0.10 | 5.69 | 0.12 | 6.01 | 0.11 | 6.14 | 0.12 | 7.83 | 0.12 |
| 388.2 | 2.70 | 0.02 | 3.42 | 0.02 | 3.05 | 0.02 | 4.17 | 0.03 | 3.70 | 0.03 | 4.66 | 0.03 | 5.25 | 0.04 |
| 398.2 | 2.76 | 0.02 | 3.36 | 0.02 | 2.93 | 0.02 | 4.05 | 0.03 | 3.52 | 0.02 | 4.52 | 0.03 | 4.86 | 0.03 |
| Average | 5.39 | 0.10 | 6.17 | 0.11 | 5.79 | 0.10 | 7.64 | 0.10 | 7.84 | 0.10 | 8.20 | 0.10 | 8.44 | 0.11 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 2.03 | 0.02 | 2.71 | 0.02 | 4.13 | 0.04 | 1.98 | 0.03 | 3.20 | 0.03 | 3.47 | 0.04 | 5.84 | 0.03 |
| 303.2 | 10.47 | 0.03 | 10.61 | 0.04 | 11.62 | 0.05 | 9.43 | 0.04 | 10.88 | 0.05 | 10.21 | 0.05 | 6.68 | 0.04 |
| 313.2 | 1.74 | 0.01 | 1.48 | 0.02 | 2.71 | 0.03 | 2.30 | 0.03 | 2.11 | 0.03 | 2.78 | 0.04 | 3.87 | 0.03 |
| 343.2 | 1.39 | 0.01 | 1.40 | 0.01 | 2.54 | 0.02 | 1.37 | 0.02 | 0.82 | 0.02 | 2.07 | 0.03 | 1.32 | 0.02 |
| 363.0 | 1.33 | 0.01 | 1.44 | 0.01 | 2.78 | 0.02 | 1.40 | 0.03 | 1.12 | 0.03 | 2.32 | 0.03 | 1.10 | 0.02 |
| 373.1 | 2.11 | 0.02 | 2.59 | 0.02 | 3.35 | 0.03 | 2.63 | 0.03 | 1.88 | 0.03 | 3.64 | 0.04 | 3.00 | 0.03 |
| 412.6 | 1.41 |  | 1.40 |  | 2.20 |  | 1.13 |  | 1.52 |  | 1.67 |  | 0.83 |  |
| 443.2 | 1.96 |  | 1.90 |  | 2.51 |  | 1.42 |  | 2.09 |  | 1.54 |  | 1.30 |  |
| 483.2 | 1.25 |  | 1.21 |  | 1.64 |  | 0.97 |  | 1.25 |  | 1.22 |  | 1.08 |  |
| Average | 2.63 | 0.02 | 2.75 | 0.02 | 3.72 | 0.03 | 2.51 | 0.03 | 2.76 | 0.03 | 3.21 | 0.04 | 2.78 | 0.03 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 19.16 | 0.02 | 19.28 | 0.02 | 16.68 | 0.03 | 18.23 | 0.02 | 19.62 | 0.02 | 17.45 | 0.03 | 15.22 | 0.01 |
| 313.1 | 6.49 | 0.02 | 6.29 | 0.02 | 8.54 | 0.02 | 7.22 | 0.02 | 6.30 | 0.02 | 8.51 | 0.02 | 7.87 | 0.02 |
| 343.2 | 12.04 | 0.04 | 12.20 | 0.04 | 13.38 | 0.04 | 11.67 | 0.02 | 11.07 | 0.03 | 11.93 | 0.02 | 10.27 | 0.03 |
| 373.1 | 3.77 | 0.03 | 4.27 | 0.03 | 4.63 | 0.03 | 3.11 | 0.03 | 3.73 | 0.03 | 3.71 | 0.04 | 1.91 | 0.03 |
| 423.2 | 6.95 | 0.07 | 7.28 | 0.07 | 6.72 | 0.07 | 5.26 | 0.05 | 6.15 | 0.05 | 5.34 | 0.06 | 6.32 | 0.05 |
| 453.2 | 7.34 | 0.10 | 7.85 | 0.10 | 6.85 | 0.11 | 5.22 | 0.09 | 6.41 | 0.09 | 4.29 | 0.09 | 6.38 | 0.08 |
| 483.2 | 6.08 | 0.15 | 7.05 | 0.15 | 6.23 | 0.15 | 4.04 | 0.13 | 5.02 | 0.13 | 3.53 | 0.13 | 5.08 | 0.12 |
| Average | 8.83 | 0.06 | 9.17 | 0.06 | 9.00 | 0.06 | 7.82 | 0.05 | 8.33 | 0.05 | 7.82 | 0.06 | 7.58 | 0.05 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 7.18 | 0.05 | 7.02 | 0.05 | 11.55 | 0.06 | 6.99 | 0.06 | 8.06 | 0.05 | 13.14 | 0.05 | 4.80 | 0.06 |
| Average | 7.18 | 0.05 | 7.02 | 0.05 | 11.55 | 0.06 | 6.99 | 0.06 | 8.06 | 0.05 | 13.14 | 0.05 | 4.80 | 0.06 |
|  | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *P* / bar | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* | *T* | *y1* |
| 0.1333 | 2.20 | 0.04 | 2.22 | 0.04 | 4.17 | 0.04 | 1.03 | 0.02 | 1.45 | 0.03 | 2.35 | 0.02 | 1.13 | 0.03 |
| 0.5333 | 2.06 | 0.03 | 2.30 | 0.03 | 1.82 | 0.02 | 1.09 | 0.02 | 1.34 | 0.02 | 1.69 | 0.02 | 0.97 | 0.02 |
| 1.0132 | 2.02 | 0.03 | 2.07 | 0.03 | 1.49 | 0.02 | 0.88 | 0.01 | 1.02 | 0.02 | 1.51 | 0.02 | 0.90 | 0.01 |
| Average | 2.09 | 0.03 | 2.19 | 0.03 | 2.49 | 0.02 | 1.00 | 0.02 | 1.27 | 0.02 | 1.85 | 0.02 | 1.00 | 0.02 |
| Overall average | 5.43 | 0.06 | 5.81 | 0.07 | 6.17 | 0.07 | 5.82 | 0.06 | 6.16 | 0.06 | 6.49 | 0.07 | 6.02 | 0.06 |
| a Overall average values computed from isothermal data only.  b Values for CPA-CR1 2B-2B taken from ([Román-Ramírez and Leeke 2020](#_ENREF_20)), except isobaric data. | | | | | | | | | | | | | | | |

Table S4. Values of the binary interaction parameter () for the organic acid + water systems with the different EoS studied.a

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-CR1 |  |  |  |  |  |  |  | PC-SAFT |  |  |  |  |  |  |  |
| formic acid |  |  |  |  |  |  |  | formic acid |  |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.1 | -0.135 | -0.051 | -0.202 | -0.253 | -0.345 | -0.305 |  | 303.1 | -0.014 | 0.077 | -0.005 | -0.119 | -0.094 | -0.118 | -0.032 |
| 318.1 | -0.131 | -0.044 | -0.202 | -0.261 | -0.367 | -0.326 |  | 318.1 | -0.008 | 0.075 | -0.012 | -0.120 | -0.092 | -0.125 | -0.036 |
| 323.1 | -0.137 | -0.050 | -0.220 | -0.267 | -0.331 | -0.331 |  | 323.1 | -0.014 | 0.074 | -0.020 | -0.122 | -0.095 | -0.123 | -0.037 |
| 328.1 | -0.122 | -0.042 | -0.207 | -0.245 | -0.313 | -0.303 |  | 328.1 | -0.007 | 0.078 | -0.005 | -0.108 | -0.081 | -0.110 | -0.030 |
| 333.1 | -0.122 | -0.036 | -0.207 | -0.249 | -0.333 | -0.312 |  | 333.1 | -0.008 | 0.075 | -0.008 | -0.109 | -0.082 | -0.113 | -0.031 |
| 353.1 | -0.111 | -0.028 | -0.209 | -0.252 | -0.353 | -0.329 |  | 353.1 | -0.006 | 0.069 | -0.023 | -0.108 | -0.077 | -0.118 | -0.033 |
| 388.2 | -0.107 | -0.033 | -0.226 | -0.236 | -0.325 | -0.299 |  | 388.2 | 0.002 | 0.079 | -0.015 | -0.090 | -0.062 | -0.098 | -0.023 |
| 398.2 | -0.099 | -0.026 | -0.220 | -0.222 | -0.299 | -0.299 |  | 398.2 | 0.004 | 0.082 | -0.010 | -0.083 | -0.053 | -0.094 | -0.018 |
| acetic acid |  |  |  |  |  |  |  | acetic acid |  |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 293.2 | -0.157 | -0.075 | -0.178 | -0.207 | -0.183 | -0.173 |  | 293.2 | 0.028 | 0.108 | 0.031 | -0.050 | -0.032 | -0.044 | -0.034 |
| 303.2 | -0.186 | -0.107 | -0.218 | -0.229 | -0.220 | -0.226 |  | 303.2 | 0.011 | 0.093 | 0.008 | -0.068 | -0.046 | -0.069 | -0.043 |
| 313.2 | -0.145 | -0.064 | -0.182 | -0.189 | -0.170 | -0.168 |  | 313.2 | 0.035 | 0.112 | 0.033 | -0.041 | -0.022 | -0.036 | -0.030 |
| 343.2 | -0.159 | -0.089 | -0.211 | -0.193 | -0.171 | -0.182 |  | 343.2 | 0.035 | 0.110 | 0.039 | -0.037 | -0.015 | -0.035 | -0.030 |
| 363.0 | -0.128 | -0.061 | -0.204 | -0.173 | -0.162 | -0.165 |  | 363.0 | 0.045 | 0.116 | 0.035 | -0.024 | -0.004 | -0.028 | -0.024 |
| 373.1 | -0.112 | -0.045 | -0.197 | -0.153 | -0.134 | -0.150 |  | 373.1 | 0.049 | 0.117 | 0.033 | -0.018 | 0.003 | -0.029 | -0.020 |
| 412.6 | -0.117 | -0.060 | -0.220 | -0.145 | -0.125 | -0.148 |  | 412.6 | 0.056 | 0.123 | 0.046 | -0.007 | 0.016 | -0.010 | -0.012 |
| 443.2 | -0.107 | -0.055 | -0.226 | -0.133 | -0.118 | -0.140 |  | 443.2 | 0.061 | 0.128 | 0.052 | 0.001 | 0.028 | -0.001 | -0.003 |
| 483.2 | -0.083 | -0.038 | -0.240 | -0.108 | -0.088 | -0.140 |  | 483.2 | 0.066 | 0.128 | 0.046 | 0.010 | 0.035 | -0.002 | 0.008 |
| propanoic acid |  |  |  |  |  |  |  | propanoic acid | |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.2 | -0.213 | -0.147 | -0.263 | -0.233 | -0.246 | -0.211 |  | 303.2 | -0.008 | 0.057 | -0.016 | -0.038 | -0.016 | -0.041 | -0.047 |
| 313.1 | -0.167 | -0.109 | -0.165 | -0.182 | -0.201 | -0.111 |  | 313.1 | 0.028 | 0.086 | 0.032 | 0.005 | 0.022 | 0.016 | -0.024 |
| 343.2 | -0.131 | -0.080 | -0.138 | -0.147 | -0.116 | -0.067 |  | 343.2 | 0.049 | 0.102 | 0.042 | 0.028 | 0.041 | 0.034 | -0.011 |
| 373.1 | -0.086 | -0.052 | -0.162 | -0.134 | -0.117 | -0.080 |  | 373.1 | 0.050 | 0.098 | 0.032 | 0.035 | 0.046 | 0.025 | -0.004 |
| 423.2 | -0.096 | -0.054 | -0.178 | -0.096 | -0.075 | -0.065 |  | 423.2 | 0.060 | 0.105 | 0.038 | 0.045 | 0.057 | 0.040 | 0.009 |
| 453.2 | -0.042 | -0.030 | -0.172 | -0.045 | -0.029 | -0.024 |  | 453.2 | 0.075 | 0.115 | 0.037 | 0.060 | 0.075 | 0.042 | 0.018 |
| 483.2 | -0.008 | 0.030 | -0.145 | -0.010 | 0.010 | 0.006 |  | 483.2 | 0.087 | 0.123 | 0.044 | 0.072 | 0.088 | 0.056 | 0.036 |
| butanoic acid |  |  |  |  |  |  |  | butanoic acid | |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.2 | -0.186 | -0.138 | -0.236 | -0.215 | -0.220 | -0.192 |  | 303.2 | -0.005 | 0.047 | -0.033 | -0.017 | -0.001 | -0.026 | -0.048 |

Table S4. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-ECR |  |  |  |  |  |  |  | PCP-SAFT |  |  |  |  |  |  |  |
| formic acid |  |  |  |  |  |  |  | formic acid |  |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.1 | -0.141 | -0.055 | -0.213 | -0.262 | -0.349 | -0.323 |  | 303.1 | -0.057 | -0.009 | -0.093 | -0.188 | -0.172 | -0.204 | -0.045 |
| 318.1 | -0.138 | -0.057 | -0.213 | -0.271 | -0.372 | -0.349 |  | 318.1 | -0.058 | -0.017 | -0.081 | -0.194 | -0.176 | -0.214 | -0.052 |
| 323.1 | -0.143 | -0.056 | -0.230 | -0.276 | -0.336 | -0.349 |  | 323.1 | -0.064 | -0.005 | -0.089 | -0.189 | -0.149 | -0.205 | -0.047 |
| 328.1 | -0.130 | -0.047 | -0.213 | -0.255 | -0.320 | -0.324 |  | 328.1 | -0.049 | -0.009 | -0.069 | -0.177 | -0.137 | -0.194 | -0.042 |
| 333.1 | -0.129 | -0.045 | -0.222 | -0.260 | -0.340 | -0.336 |  | 333.1 | -0.050 | -0.004 | -0.073 | -0.181 | -0.162 | -0.199 | -0.045 |
| 353.1 | -0.119 | -0.039 | -0.224 | -0.265 | -0.361 | -0.360 |  | 353.1 | -0.058 | -0.004 | -0.087 | -0.184 | -0.162 | -0.205 | -0.051 |
| 388.2 | -0.114 | -0.039 | -0.240 | -0.248 | -0.325 | -0.321 |  | 388.2 | -0.038 | 0.017 | -0.067 | -0.162 | -0.142 | -0.179 | -0.032 |
| 398.2 | -0.105 | -0.032 | -0.236 | -0.237 | -0.306 | -0.333 |  | 398.2 | -0.030 | 0.024 | -0.060 | -0.155 | -0.132 | -0.172 | -0.027 |
| acetic acid |  |  |  |  |  |  |  | acetic acid |  |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 293.2 | -0.171 | -0.094 | -0.204 | -0.227 | -0.208 | -0.220 |  | 293.2 | -0.043 | 0.012 | -0.064 | -0.119 | -0.097 | -0.140 | -0.045 |
| 303.2 | -0.198 | -0.124 | -0.260 | -0.256 | -0.246 | -0.281 |  | 303.2 | -0.059 | 0.015 | -0.087 | -0.140 | -0.122 | -0.163 | -0.063 |
| 313.2 | -0.159 | -0.084 | -0.202 | -0.215 | -0.206 | -0.217 |  | 313.2 | -0.031 | 0.018 | -0.059 | -0.108 | -0.088 | -0.128 | -0.044 |
| 343.2 | -0.162 | -0.092 | -0.228 | -0.214 | -0.201 | -0.238 |  | 343.2 | -0.020 | 0.026 | -0.046 | -0.101 | -0.079 | -0.123 | -0.044 |
| 363.0 | -0.145 | -0.078 | -0.226 | -0.201 | -0.188 | -0.221 |  | 363.0 | -0.011 | 0.037 | -0.040 | -0.090 | -0.067 | -0.108 | -0.038 |
| 373.1 | -0.132 | -0.067 | -0.229 | -0.190 | -0.170 | -0.228 |  | 373.1 | -0.009 | 0.039 | -0.041 | -0.089 | -0.066 | -0.110 | -0.036 |
| 412.6 | -0.129 | -0.073 | -0.238 | -0.176 | -0.161 | -0.210 |  | 412.6 | 0.011 | 0.058 | -0.016 | -0.064 | -0.042 | -0.078 | -0.024 |
| 443.2 | -0.119 | -0.068 | -0.234 | -0.160 | -0.143 | -0.200 |  | 443.2 | 0.024 | 0.069 | -0.001 | -0.049 | -0.029 | -0.064 | -0.014 |
| 483.2 | -0.098 | -0.053 | -0.261 | -0.146 | -0.127 | -0.211 |  | 483.2 | 0.032 | 0.075 | -0.002 | -0.041 | -0.019 | -0.056 | -0.005 |
| propanoic acid |  |  |  |  |  |  |  | propanoic acid | |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.2 | -0.235 | -0.170 | -0.278 | -0.272 | -0.264 | -0.281 |  | 303.2 | -0.079 | -0.035 | -0.133 | -0.120 | -0.092 | -0.151 | -0.071 |
| 313.1 | -0.174 | -0.112 | -0.178 | -0.203 | -0.207 | -0.163 |  | 313.1 | -0.031 | 0.006 | -0.073 | -0.061 | -0.048 | -0.088 | -0.039 |
| 343.2 | -0.135 | -0.090 | -0.155 | -0.165 | -0.168 | -0.124 |  | 343.2 | -0.009 | 0.028 | -0.044 | -0.045 | -0.026 | -0.071 | -0.024 |
| 373.1 | -0.098 | -0.074 | -0.193 | -0.158 | -0.168 | -0.151 |  | 373.1 | -0.013 | 0.020 | -0.061 | -0.046 | -0.027 | -0.075 | -0.026 |
| 423.2 | -0.113 | -0.070 | -0.200 | -0.142 | -0.129 | -0.141 |  | 423.2 | 0.002 | 0.033 | -0.036 | -0.022 | -0.005 | -0.038 | -0.010 |
| 453.2 | -0.072 | -0.031 | -0.205 | -0.106 | -0.092 | -0.137 |  | 453.2 | 0.014 | 0.044 | -0.033 | -0.014 | 0.005 | -0.033 | -0.002 |
| 483.2 | -0.042 | -0.005 | -0.194 | -0.077 | -0.060 | -0.106 |  | 483.2 | 0.029 | 0.057 | -0.018 | 0.005 | 0.025 | -0.023 | 0.014 |
| butanoic acid |  |  |  |  |  |  |  | butanoic acid | |  |  |  |  |  |  |
| *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C |  | *T* / K | 1A-2B | 1A-3B | 1A-4C | 2B-2B | 2B-3B | 2B-4C | Non-assoc. |
| 303.2 | -0.205 | -0.155 | -0.286 | -0.257 | -0.177 | -0.272 |  | 303.2 | -0.091 | -0.056 | -0.148 | -0.110 | -0.090 | -0.166 | -0.069 |
| b Values for CPA-CR1 2B-2B taken from ([Román-Ramírez and Leeke 2020](#_ENREF_20)) | | | | | | | | | | | | | | | |

Table S5. Deviations ( and ) for correlations with from TableS4.a

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-CR1 |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 4.41 | 0.11 | 6.09 | 0.12 | 4.58 | 0.11 | 9.92 | 0.12 | 11.48 | 0.14 | 10.82 | 0.12 |
| 318.1 | 4.27 | 0.11 | 5.17 | 0.12 | 6.22 | 0.11 | 8.57 | 0.12 | 8.99 | 0.14 | 9.04 | 0.13 |
| 323.1 | 5.08 | 0.14 | 5.23 | 0.14 | 4.18 | 0.13 | 8.23 | 0.14 | 7.72 | 0.15 | 8.23 | 0.14 |
| 328.1 | 4.04 | 0.13 | 4.58 | 0.13 | 3.17 | 0.13 | 7.22 | 0.13 | 5.24 | 0.15 | 7.46 | 0.13 |
| 333.1 | 2.99 | 0.10 | 3.83 | 0.11 | 2.12 | 0.10 | 6.03 | 0.11 | 6.18 | 0.13 | 6.34 | 0.11 |
| 353.1 | 1.81 | 0.09 | 2.33 | 0.09 | 2.67 | 0.08 | 3.60 | 0.11 | 4.44 | 0.12 | 3.85 | 0.11 |
| 388.2 | 0.93 | 0.01 | 1.20 | 0.01 | 1.26 | 0.02 | 2.86 | 0.02 | 1.76 | 0.01 | 3.30 | 0.03 |
| 398.2 | 0.80 | 0.02 | 1.15 | 0.01 | 1.19 | 0.02 | 2.62 | 0.02 | 1.63 | 0.01 | 3.00 | 0.02 |
| Average | 3.04 | 0.09 | 3.70 | 0.09 | 3.17 | 0.09 | 6.13 | 0.10 | 5.93 | 0.11 | 6.51 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 7.78 | 0.05 | 9.88 | 0.06 | 5.62 | 0.04 | 4.98 | 0.03 | 7.71 | 0.05 | 3.35 | 0.02 |
| 303.2 | 2.39 | 0.03 | 4.21 | 0.04 | 2.72 | 0.02 | 0.96 | 0.01 | 2.06 | 0.02 | 2.14 | 0.01 |
| 313.2 | 8.02 | 0.05 | 9.31 | 0.06 | 6.46 | 0.05 | 5.15 | 0.03 | 6.48 | 0.06 | 3.97 | 0.03 |
| 343.2 | 5.21 | 0.03 | 6.57 | 0.04 | 3.95 | 0.03 | 3.03 | 0.02 | 5.98 | 0.03 | 2.13 | 0.01 |
| 363.0 | 5.58 | 0.04 | 6.76 | 0.04 | 4.19 | 0.03 | 3.18 | 0.02 | 5.12 | 0.03 | 2.01 | 0.02 |
| 373.1 | 3.70 | 0.04 | 4.56 | 0.05 | 2.53 | 0.04 | 1.35 | 0.03 | 2.47 | 0.04 | 0.54 | 0.03 |
| 412.6 | 4.69 |  | 5.52 |  | 3.78 |  | 2.80 |  | 3.97 |  | 2.06 |  |
| 443.2 | 5.48 |  | 6.28 |  | 4.86 |  | 3.54 |  | 4.73 |  | 2.80 |  |
| 483.2 | 3.98 |  | 4.69 |  | 3.37 |  | 2.45 |  | 3.68 |  | 1.95 |  |
| Average | 5.20 | 0.04 | 6.42 | 0.05 | 4.16 | 0.03 | 3.05 | 0.02 | 4.69 | 0.04 | 2.33 | 0.02 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 11.50 | 0.07 | 9.84 | 0.07 | 5.36 | 0.06 | 7.28 | 0.05 | 19.54 | 0.06 | 4.06 | 0.04 |
| 313.1 | 11.38 | 0.05 | 14.11 | 0.05 | 8.44 | 0.03 | 10.62 | 0.03 | 15.67 | 0.04 | 8.04 | 0.03 |
| 343.2 | 15.62 | 0.08 | 17.34 | 0.09 | 13.66 | 0.07 | 13.64 | 0.06 | 10.02 | 0.06 | 11.25 | 0.05 |
| 373.1 | 9.62 | 0.03 | 13.07 | 0.05 | 7.54 | 0.03 | 9.53 | 0.03 | 8.65 | 0.05 | 6.93 | 0.03 |
| 423.2 | 12.27 | 0.09 | 13.29 | 0.09 | 10.29 | 0.09 | 10.95 | 0.07 | 10.55 | 0.06 | 9.50 | 0.07 |
| 453.2 | 13.34 | 0.12 | 13.98 | 0.12 | 11.36 | 0.13 | 10.95 | 0.10 | 12.21 | 0.10 | 9.77 | 0.10 |
| 483.2 | 11.51 | 0.17 | 12.51 | 0.17 | 10.30 | 0.17 | 8.97 | 0.15 | 10.22 | 0.15 | 8.26 | 0.15 |
| Average | 12.18 | 0.09 | 13.45 | 0.09 | 9.56 | 0.08 | 10.28 | 0.07 | 12.41 | 0.07 | 8.26 | 0.07 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 12.80 | 0.04 | 16.68 | 0.04 | 10.14 | 0.04 | 11.24 | 0.05 | 12.57 | 0.05 | 7.13 | 0.05 |
| Average | 12.80 | 0.04 | 16.68 | 0.04 | 10.14 | 0.04 | 11.24 | 0.05 | 12.57 | 0.05 | 7.13 | 0.05 |
| Overall average | 6.77 | 0.07 | 7.93 | 0.08 | 5.60 | 0.07 | 6.39 | 0.07 | 7.56 | 0.08 | 5.52 | 0.07 |

Table S5. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CPA-ECR |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 4.56 | 0.11 | 5.93 | 0.12 | 4.31 | 0.12 | 10.15 | 0.12 | 11.17 | 0.14 | 11.52 | 0.13 |
| 318.1 | 4.27 | 0.11 | 5.08 | 0.12 | 4.90 | 0.11 | 8.78 | 0.13 | 8.82 | 0.14 | 9.60 | 0.13 |
| 323.1 | 5.25 | 0.14 | 5.67 | 0.14 | 4.67 | 0.13 | 8.41 | 0.14 | 7.34 | 0.15 | 8.75 | 0.14 |
| 328.1 | 3.93 | 0.13 | 4.67 | 0.13 | 3.88 | 0.13 | 7.37 | 0.13 | 5.08 | 0.15 | 7.92 | 0.13 |
| 333.1 | 2.89 | 0.11 | 3.60 | 0.11 | 2.66 | 0.11 | 6.24 | 0.11 | 5.88 | 0.13 | 6.92 | 0.12 |
| 353.1 | 1.42 | 0.09 | 1.42 | 0.09 | 1.36 | 0.08 | 3.73 | 0.11 | 4.40 | 0.12 | 4.30 | 0.12 |
| 388.2 | 0.72 | 0.01 | 0.64 | 0.01 | 1.13 | 0.02 | 3.07 | 0.02 | 1.71 | 0.01 | 3.91 | 0.03 |
| 398.2 | 0.59 | 0.01 | 0.57 | 0.01 | 1.04 | 0.02 | 2.81 | 0.02 | 1.86 | 0.01 | 3.55 | 0.03 |
| Average | 2.96 | 0.09 | 3.45 | 0.09 | 2.99 | 0.09 | 6.32 | 0.10 | 5.78 | 0.11 | 7.06 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 5.95 | 0.04 | 7.12 | 0.05 | 3.15 | 0.02 | 3.63 | 0.02 | 6.03 | 0.04 | 1.78 | 0.02 |
| 303.2 | 1.51 | 0.02 | 9.65 | 0.03 | 2.65 | 0.02 | 2.01 | 0.01 | 0.73 | 0.01 | 4.54 | 0.02 |
| 313.2 | 6.20 | 0.04 | 6.89 | 0.05 | 3.82 | 0.03 | 4.05 | 0.03 | 6.76 | 0.04 | 1.89 | 0.03 |
| 343.2 | 3.84 | 0.03 | 4.86 | 0.03 | 2.55 | 0.02 | 2.10 | 0.01 | 4.86 | 0.02 | 1.04 | 0.01 |
| 363.0 | 4.12 | 0.03 | 4.87 | 0.03 | 2.51 | 0.02 | 2.15 | 0.02 | 3.49 | 0.03 | 0.89 | 0.02 |
| 373.1 | 2.22 | 0.03 | 2.60 | 0.03 | 0.90 | 0.04 | 0.70 | 0.02 | 1.27 | 0.03 | 2.00 | 0.03 |
| 412.6 | 3.65 |  | 4.23 |  | 2.37 |  | 2.08 |  | 2.91 |  | 0.80 |  |
| 443.2 | 4.42 |  | 4.96 |  | 3.31 |  | 2.69 |  | 3.56 |  | 1.37 |  |
| 483.2 | 3.05 |  | 3.55 |  | 2.10 |  | 1.70 |  | 2.39 |  | 0.80 |  |
| Average | 3.88 | 0.03 | 5.41 | 0.04 | 2.59 | 0.02 | 2.34 | 0.02 | 3.56 | 0.03 | 1.68 | 0.02 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 6.01 | 0.05 | 8.80 | 0.06 | 3.98 | 0.03 | 3.75 | 0.04 | 13.17 | 0.04 | 2.93 | 0.02 |
| 313.1 | 9.26 | 0.03 | 11.54 | 0.04 | 4.57 | 0.01 | 7.91 | 0.03 | 7.13 | 0.03 | 3.39 | 0.02 |
| 343.2 | 12.33 | 0.07 | 14.08 | 0.07 | 9.32 | 0.05 | 10.57 | 0.05 | 8.77 | 0.04 | 6.23 | 0.03 |
| 373.1 | 6.30 | 0.04 | 9.13 | 0.03 | 3.92 | 0.02 | 6.08 | 0.04 | 5.75 | 0.04 | 1.67 | 0.03 |
| 423.2 | 10.50 | 0.08 | 10.97 | 0.08 | 7.37 | 0.09 | 8.95 | 0.06 | 9.75 | 0.06 | 5.78 | 0.06 |
| 453.2 | 10.73 | 0.12 | 11.22 | 0.11 | 7.74 | 0.12 | 8.67 | 0.09 | 9.46 | 0.09 | 5.55 | 0.10 |
| 483.2 | 8.97 | 0.16 | 9.47 | 0.16 | 6.67 | 0.17 | 6.86 | 0.14 | 7.57 | 0.14 | 4.35 | 0.14 |
| Average | 9.16 | 0.08 | 10.74 | 0.08 | 6.23 | 0.07 | 7.54 | 0.06 | 8.80 | 0.06 | 4.27 | 0.06 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 7.54 | 0.05 | 10.56 | 0.05 | 7.97 | 0.05 | 5.82 | 0.05 | 14.49 | 0.05 | 4.21 | 0.06 |
| Average | 7.54 | 0.05 | 10.56 | 0.05 | 7.97 | 0.05 | 5.82 | 0.05 | 14.49 | 0.05 | 4.21 | 0.06 |
| Overall average | 5.21 | 0.07 | 6.48 | 0.07 | 3.95 | 0.06 | 5.21 | 0.06 | 6.17 | 0.07 | 4.23 | 0.06 |

Table S5. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PC-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 5.70 | 0.12 | 7.83 | 0.14 | 8.23 | 0.12 | 10.15 | 0.12 | 9.06 | 0.12 | 11.44 | 0.13 | 9.53 | 0.12 |
| 318.1 | 5.61 | 0.11 | 7.29 | 0.13 | 6.94 | 0.12 | 8.30 | 0.13 | 7.37 | 0.12 | 9.28 | 0.13 | 8.66 | 0.13 |
| 323.1 | 5.53 | 0.13 | 6.78 | 0.14 | 6.20 | 0.14 | 7.54 | 0.14 | 6.57 | 0.14 | 8.53 | 0.14 | 8.02 | 0.14 |
| 328.1 | 4.67 | 0.13 | 6.50 | 0.14 | 6.06 | 0.13 | 7.01 | 0.13 | 6.16 | 0.13 | 7.78 | 0.13 | 7.87 | 0.13 |
| 333.1 | 3.38 | 0.11 | 4.98 | 0.12 | 5.09 | 0.11 | 5.64 | 0.11 | 4.77 | 0.11 | 6.71 | 0.12 | 6.66 | 0.12 |
| 353.1 | 1.32 | 0.10 | 2.65 | 0.11 | 1.74 | 0.10 | 3.73 | 0.11 | 3.04 | 0.10 | 4.37 | 0.12 | 5.17 | 0.12 |
| 388.2 | 1.30 | 0.01 | 2.66 | 0.02 | 2.49 | 0.02 | 2.98 | 0.02 | 2.15 | 0.02 | 3.92 | 0.03 | 3.62 | 0.03 |
| 398.2 | 1.38 | 0.01 | 2.58 | 0.02 | 2.38 | 0.02 | 2.75 | 0.02 | 2.01 | 0.02 | 3.62 | 0.03 | 3.38 | 0.03 |
| Average | 3.61 | 0.09 | 5.16 | 0.10 | 4.89 | 0.09 | 6.01 | 0.10 | 5.14 | 0.10 | 6.96 | 0.10 | 6.62 | 0.10 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 2.87 | 0.02 | 1.20 | 0.01 | 2.81 | 0.03 | 2.58 | 0.02 | 2.37 | 0.03 | 1.64 | 0.02 | 5.90 | 0.04 |
| 303.2 | 2.04 | 0.02 | 3.60 | 0.03 | 6.10 | 0.04 | 2.78 | 0.01 | 2.58 | 0.01 | 5.44 | 0.03 | 1.33 | 0.01 |
| 313.2 | 3.29 | 0.02 | 1.18 | 0.01 | 2.18 | 0.02 | 3.23 | 0.03 | 3.44 | 0.03 | 1.48 | 0.03 | 5.17 | 0.04 |
| 343.2 | 1.80 | 0.01 | 0.72 | 0.00 | 2.06 | 0.02 | 1.70 | 0.01 | 1.93 | 0.01 | 1.33 | 0.02 | 2.62 | 0.01 |
| 363.0 | 1.78 | 0.01 | 0.40 | 0.00 | 2.27 | 0.02 | 1.48 | 0.02 | 1.82 | 0.02 | 1.34 | 0.02 | 2.35 | 0.02 |
| 373.1 | 0.54 | 0.02 | 1.67 | 0.02 | 2.46 | 0.03 | 0.69 | 0.02 | 0.44 | 0.03 | 2.46 | 0.03 | 1.23 | 0.02 |
| 412.6 | 2.05 |  | 1.11 |  | 1.83 |  | 1.61 |  | 2.32 |  | 1.02 |  | 2.61 |  |
| 443.2 | 2.75 |  | 1.84 |  | 2.12 |  | 2.11 |  | 2.84 |  | 1.25 |  | 2.90 |  |
| 483.2 | 1.75 |  | 1.02 |  | 1.38 |  | 1.24 |  | 1.56 |  | 0.80 |  | 2.06 |  |
| Average | 2.10 | 0.02 | 1.41 | 0.01 | 2.58 | 0.03 | 1.93 | 0.02 | 2.14 | 0.02 | 1.86 | 0.03 | 2.91 | 0.02 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 4.62 | 0.05 | 5.60 | 0.04 | 4.30 | 0.03 | 2.90 | 0.04 | 5.79 | 0.04 | 4.08 | 0.02 | 3.77 | 0.04 |
| 313.1 | 8.49 | 0.03 | 9.47 | 0.03 | 3.74 | 0.01 | 10.19 | 0.05 | 7.25 | 0.03 | 2.73 | 0.02 | 8.47 | 0.03 |
| 343.2 | 11.34 | 0.06 | 11.27 | 0.06 | 8.65 | 0.04 | 9.45 | 0.04 | 9.08 | 0.04 | 5.99 | 0.03 | 10.25 | 0.05 |
| 373.1 | 6.91 | 0.03 | 6.68 | 0.03 | 3.75 | 0.03 | 4.65 | 0.04 | 5.35 | 0.04 | 2.02 | 0.03 | 6.35 | 0.04 |
| 423.2 | 9.42 | 0.08 | 9.08 | 0.07 | 6.75 | 0.08 | 8.09 | 0.06 | 8.67 | 0.06 | 5.34 | 0.06 | 9.77 | 0.05 |
| 453.2 | 9.68 | 0.11 | 9.26 | 0.11 | 7.08 | 0.11 | 7.87 | 0.09 | 8.50 | 0.09 | 5.18 | 0.09 | 9.26 | 0.08 |
| 483.2 | 8.18 | 0.16 | 7.82 | 0.15 | 6.22 | 0.16 | 6.27 | 0.14 | 6.71 | 0.14 | 4.10 | 0.14 | 7.65 | 0.12 |
| Average | 8.38 | 0.07 | 8.45 | 0.07 | 5.78 | 0.07 | 7.06 | 0.06 | 7.34 | 0.06 | 4.21 | 0.05 | 7.93 | 0.06 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 6.59 | 0.05 | 8.72 | 0.05 | 7.65 | 0.05 | 4.55 | 0.05 | 5.71 | 0.05 | 4.58 | 0.06 | 6.58 | 0.05 |
| Average | 6.59 | 0.05 | 8.72 | 0.05 | 7.65 | 0.05 | 4.55 | 0.05 | 5.71 | 0.05 | 4.58 | 0.06 | 6.58 | 0.05 |
| Overall average | 4.52 | 0.06 | 4.88 | 0.07 | 4.42 | 0.06 | 4.78 | 0.06 | 4.70 | 0.06 | 4.26 | 0.06 | 5.65 | 0.06 |

Table S5. Continuation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PCP-SAFT |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| formic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.1 | 8.66 | 0.12 | 9.31 | 0.14 | 8.78 | 0.14 | 12.24 | 0.13 | 12.46 | 0.13 | 13.04 | 0.13 | 11.81 | 0.13 |
| 318.1 | 7.30 | 0.12 | 7.97 | 0.14 | 8.08 | 0.13 | 9.87 | 0.13 | 9.90 | 0.13 | 10.46 | 0.14 | 10.45 | 0.14 |
| 323.1 | 6.64 | 0.14 | 7.65 | 0.14 | 7.13 | 0.14 | 9.03 | 0.14 | 11.90 | 0.13 | 9.59 | 0.14 | 9.71 | 0.14 |
| 328.1 | 6.42 | 0.13 | 7.04 | 0.15 | 7.01 | 0.13 | 8.18 | 0.13 | 11.65 | 0.12 | 8.70 | 0.13 | 8.86 | 0.13 |
| 333.1 | 5.31 | 0.11 | 6.02 | 0.13 | 6.12 | 0.11 | 7.19 | 0.12 | 6.59 | 0.12 | 7.80 | 0.12 | 8.27 | 0.12 |
| 353.1 | 2.07 | 0.11 | 2.80 | 0.12 | 2.05 | 0.11 | 4.63 | 0.12 | 4.56 | 0.12 | 4.95 | 0.12 | 5.74 | 0.13 |
| 388.2 | 2.70 | 0.02 | 3.39 | 0.02 | 3.00 | 0.02 | 4.17 | 0.03 | 3.40 | 0.03 | 4.67 | 0.03 | 5.27 | 0.04 |
| 398.2 | 2.62 | 0.02 | 3.23 | 0.02 | 2.84 | 0.02 | 3.90 | 0.03 | 3.20 | 0.02 | 4.35 | 0.03 | 4.93 | 0.03 |
| Average | 5.21 | 0.10 | 5.93 | 0.11 | 5.63 | 0.10 | 7.40 | 0.10 | 7.96 | 0.10 | 7.94 | 0.10 | 8.13 | 0.11 |
| acetic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 293.2 | 2.15 | 0.02 | 2.74 | 0.02 | 4.16 | 0.04 | 1.92 | 0.03 | 3.14 | 0.03 | 3.34 | 0.04 | 3.04 | 0.05 |
| 303.2 | 5.51 | 0.03 | 10.61 | 0.04 | 7.71 | 0.05 | 5.84 | 0.03 | 5.73 | 0.03 | 7.47 | 0.05 | 3.43 | 0.02 |
| 313.2 | 1.61 | 0.01 | 1.47 | 0.02 | 2.76 | 0.03 | 1.64 | 0.03 | 2.10 | 0.04 | 2.07 | 0.04 | 2.79 | 0.04 |
| 343.2 | 1.38 | 0.01 | 1.29 | 0.01 | 2.53 | 0.02 | 1.45 | 0.02 | 1.08 | 0.02 | 2.04 | 0.02 | 0.71 | 0.01 |
| 363.0 | 1.28 | 0.01 | 1.41 | 0.01 | 2.78 | 0.02 | 1.40 | 0.02 | 1.22 | 0.03 | 2.31 | 0.03 | 0.66 | 0.02 |
| 373.1 | 1.97 | 0.02 | 2.46 | 0.02 | 2.85 | 0.03 | 2.51 | 0.03 | 1.36 | 0.03 | 3.32 | 0.03 | 2.37 | 0.02 |
| 412.6 | 1.11 |  | 0.95 |  | 1.98 |  | 1.00 |  | 1.26 |  | 1.58 |  | 0.81 |  |
| 443.2 | 1.71 |  | 1.56 |  | 2.13 |  | 1.23 |  | 1.85 |  | 1.71 |  | 1.19 |  |
| 483.2 | 0.88 |  | 0.87 |  | 1.44 |  | 0.78 |  | 1.02 |  | 1.02 |  | 0.77 |  |
| Average | 1.96 | 0.02 | 2.60 | 0.02 | 3.15 | 0.03 | 1.97 | 0.03 | 2.09 | 0.03 | 2.76 | 0.04 | 1.75 | 0.03 |
| propanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 3.64 | 0.03 | 3.19 | 0.03 | 7.87 | 0.03 | 5.56 | 0.02 | 5.41 | 0.02 | 10.01 | 0.02 | 3.05 | 0.03 |
| 313.1 | 4.15 | 0.01 | 4.50 | 0.02 | 4.40 | 0.02 | 2.29 | 0.02 | 3.16 | 0.02 | 3.02 | 0.03 | 3.70 | 0.01 |
| 343.2 | 7.81 | 0.04 | 8.44 | 0.04 | 9.22 | 0.03 | 6.50 | 0.02 | 6.38 | 0.03 | 7.22 | 0.03 | 5.64 | 0.03 |
| 373.1 | 3.14 | 0.03 | 3.79 | 0.03 | 4.55 | 0.03 | 2.25 | 0.03 | 3.14 | 0.03 | 3.68 | 0.04 | 1.75 | 0.03 |
| 423.2 | 6.89 | 0.07 | 7.46 | 0.07 | 6.58 | 0.07 | 5.19 | 0.05 | 6.13 | 0.05 | 4.59 | 0.05 | 6.17 | 0.05 |
| 453.2 | 7.13 | 0.10 | 7.91 | 0.10 | 6.59 | 0.11 | 5.00 | 0.09 | 6.18 | 0.09 | 4.08 | 0.09 | 6.12 | 0.08 |
| 483.2 | 6.03 | 0.15 | 6.88 | 0.15 | 5.96 | 0.15 | 3.88 | 0.13 | 4.97 | 0.13 | 3.19 | 0.13 | 5.07 | 0.12 |
| Average | 5.54 | 0.06 | 6.02 | 0.06 | 6.45 | 0.06 | 4.38 | 0.05 | 5.05 | 0.05 | 5.11 | 0.06 | 4.50 | 0.05 |
| butanoic acid | 1A-2B | | 1A-3B | | 1A-4C | | 2B-2B | | 2B-3B | | 2B-4C | | Non-assoc. | |
| *T* / K | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* | *P* / % | *y1* |
| 303.2 | 7.18 | 0.05 | 7.02 | 0.05 | 11.55 | 0.06 | 6.99 | 0.06 | 8.06 | 0.05 | 13.14 | 0.05 | 4.80 | 0.06 |
| Average | 7.18 | 0.05 | 7.02 | 0.05 | 11.55 | 0.06 | 6.99 | 0.06 | 8.06 | 0.05 | 13.14 | 0.05 | 4.80 | 0.06 |
| Overall average | 4.21 | 0.06 | 4.80 | 0.07 | 5.20 | 0.07 | 4.59 | 0.06 | 5.04 | 0.06 | 5.49 | 0.07 | 4.68 | 0.06 |
| b Values for CPA-CR1 2B-2B taken from ([Román-Ramírez and Leeke 2020](#_ENREF_20)) | | | | | | | | | | | | | | |

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