Supplementary Materials for

# Graph Neural Networks for the prediction of infinite dilution activity coefficients

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## S1 Composition density of train/test data sets

In this work the data was randomly split into a train set and a test set with the proportion 80:20, respectively. Figure S1 shows the composition density of the complete data set and the respective train and test splits used in this work. It can be seen that a similar distribution on the infinite dilution activity coefficients values is being followed by the splits. This strengthens the interpretation of the results reported for the test set as they lie in a similar range compared to the train set. In this work, we focus on studying the interpolation performance of the proposed model instead of focusing on its extrapolation capabilities in which case a better split can be used (e.g., scaffold splitting[1]).

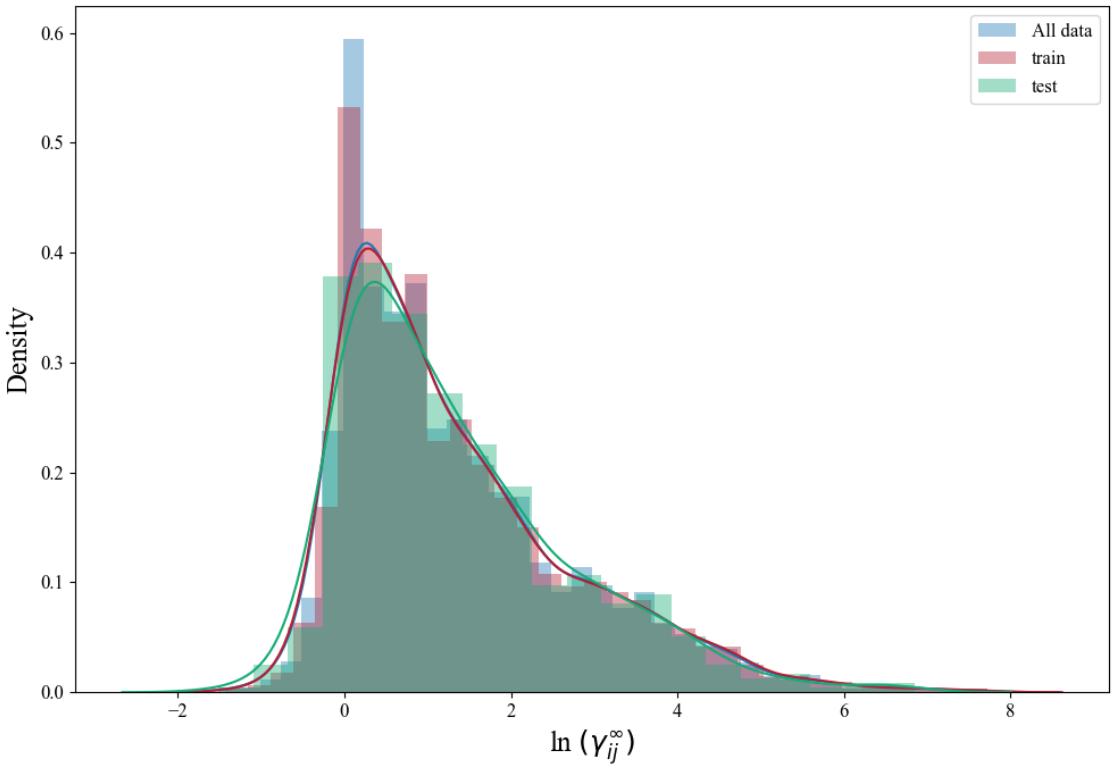


**Figure S1:** Distribution of the infinite dilution activity coefficients considered in the complete data set and the train and test splits used in this work.

## S2 Hyperparameters tuning

The hyperparameters of the proposed GNN-based model can be classified into the ones that were set based on expert knowledge (Table S1) and the ones that were actually included into the tuning (Table S2).

**Table S1:** Fixed hyperparameter values in this work based on expert knowledge.

| Hyperparameter | Value |
|---|---|
| Number of hidden layers in the (after global pooling) final MLP | 2 |
| Number of epochs | 200 |
| Batch size | 32 |

**Table S2:** Hyperparameters determined by Bayesian optimization and their corresponding bounds within the optimization problem.

| Hyperparameter | Value |
|---|---|
| Learning rate | Categorical(0.0001, 0.001, 0.01) |
| Drop out probability | Categorical(0.05, 0.1, 0.3, 0.5) |
| Number of convolutional layers | Integer(low=2, high=5) |
| Convolutional hidden state dimensions | Integer(low=16, high=64) |
| Neurons in hidden layer of the edges MLP $\phi_E$ | Integer(low=16, high=64) |
| Neurons in first hidden layer of final MLP | Integer(low=32, high=64) |
| Neurons in second hidden layer of final MLP | Integer(low=16, high=32) |

### S2.1 Bayesian Optimization

The rest of hyperparameters that were not fixed by expert knowledge were determined solving a Bayesian optimization problem. Here, a Gaussian process was trained using 7 initial samples distributed according to a Sobol sequence. The acquisition function used was Expected Improvement, which can be written under the Gaussian process as:

$$EI(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi)\,\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma > 0 \\ 0 & \text{if } \sigma = 0 \end{cases} \tag{S1}$$

where $\mathbf{x}$ denotes the set of hyperparameters; $\mu(\cdot)$ and $\sigma(\cdot)$ refer to the Gaussian process mean and standard deviation prediction, respectively; the superscript $+$ denotes the "best" $\mathbf{x}$ that has been sampled so far (i.e., $\mathbf{x}^+ = \text{argmax} f(\mathbf{x})$); $f(\cdot)$ refers to the objective function to be maximized (in this work, the negative of the mean absolute error (MAE) of the predictions on the validation data set); $\Phi(\cdot)$ and $\phi(\cdot)$

denote the cumulative distribution function and the probability density function, respectively; $\xi$ is the exploration parameter defined in this work as 0.01; and $Z$ is defined by

$$Z = \begin{cases} \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})} & \text{if } \sigma > 0 \\ 0 & \text{if } \sigma = 0 \end{cases} \tag{S2}$$

The number of calls to the $EI$ function was set to 70. Therefore, a total of 77 combinations of hyperparameters were actually visited, from where 7 were defined by the initial Sobol sampling and the remaining 70 were guided by the optimization. At each iteration, the GNN-based model was trained on a different random split for train/validation keeping the proportion 90:10 constant. Finally, the hyperparameters leading to the lowest validation mean absolute error (MAE) were selected (Table S3).

**Table S3:** Optimal hyperparameters selected from the Bayesian optimization.

| **Hyperparameter** | **Value** |
|---|---|
| Learning rate | 0.001 |
| Drop out probability | 0.1 |
| Number of convolutional layers | 5 |
| Convolutional hidden state dimensions | 30 |
| Neurons in hidden layer of the edges MLP $\phi_E$ | 64 |
| Neurons in first hidden layer of final MLP | 50 |
| Neurons in second hidden layer of final MLP | 25 |

## S3 Performance metrics

In this work, the following performance metrics were evaluated using the unscaled experimental activity coefficients $\gamma_k^\infty$ and the unscaled predicted coefficients $\gamma_{k,pred}^\infty$, where the subscript $k$ refers to the corresponding binary system of the total $N$ systems:

**Mean Absolute Error (MAE):**

$$MAE := \frac{1}{N}\sum_{k=1}^{N} \mid \gamma_k^\infty - \gamma_{k,pred}^\infty \mid \tag{S3}$$

**Standard deviation of the errors of prediction (SDEP):**

$$SDEP := \sqrt{\frac{\sum_{k=1}^{N}\left(r_k - \mu_R\right)^2}{N}} \tag{S4}$$

where $r_k := \mid \gamma_k^\infty - \gamma_{k,pred}^\infty \mid$; and $\mu_R := \frac{1}{N}\sum_{k=1}^{N} r_k$.

**Mean Squared Error (MSE):**

$$MSE := \frac{1}{N}\sum_{k=1}^{N}\left(\gamma_k^\infty - \gamma_{k,pred}^\infty\right)^2 \tag{S5}$$

**Root Mean Squared Error (RMSE):**

$$RMSE := \sqrt{\frac{1}{N}\sum_{k=1}^{N}\left(\gamma_k^\infty - \gamma_{k,pred}^\infty\right)^2} \tag{S6}$$

**Coefficient of determination ($\mathbf{R}^2$):**

$$R^2 := 1 - \frac{\sum_{k=1}^{N}\left(\gamma_k^\infty - \gamma_{k,pred}^\infty\right)^2}{\sum_{k=1}^{N}\left(\gamma_k^\infty - \mu_\gamma\right)^2} \tag{S7}$$

where $\mu_\gamma := \frac{1}{N}\sum_{k=1}^{N}\gamma_k^\infty$.

**Mean Absolute Percentage Error (MAPE):**

$$MAPE := \frac{1}{N}\sum_{k=1}^{N}\frac{\mid \gamma_k^\infty - \gamma_{k,pred}^\infty \mid}{\gamma_k^\infty} \tag{S8}$$

# S4 Additional results

## S4.1 Histograms of comparison to the GNN-based models

The following histograms show the comparison between 7 mechanistic models (the Hildebrand model was excluded due to its poor performance compared to the other ones) and the GNN single and GNN ensemble according to the mentioned metrics. The performance reported for the GNN-based models corresponds to the test set. The coverage percentage (CP) of molecules which can be predicted using the corresponding method is shown as numbers in the bars.

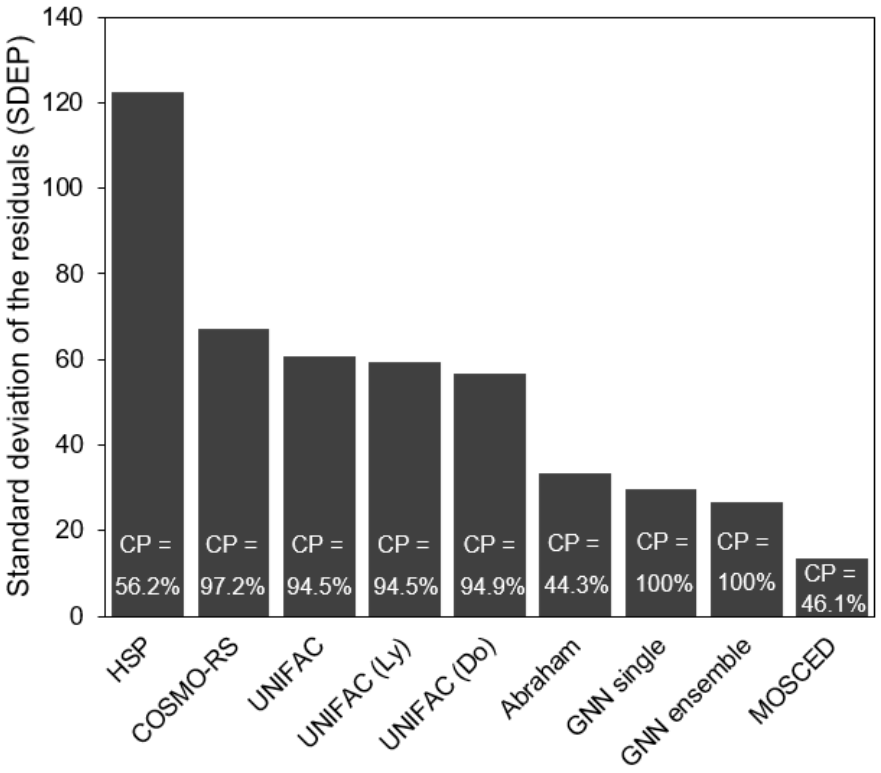


**Figure S2:** Comparison according to the Standard deviation of the errors of prediction (SDEP). The performance reported for the GNN-based models corresponds to the test set.

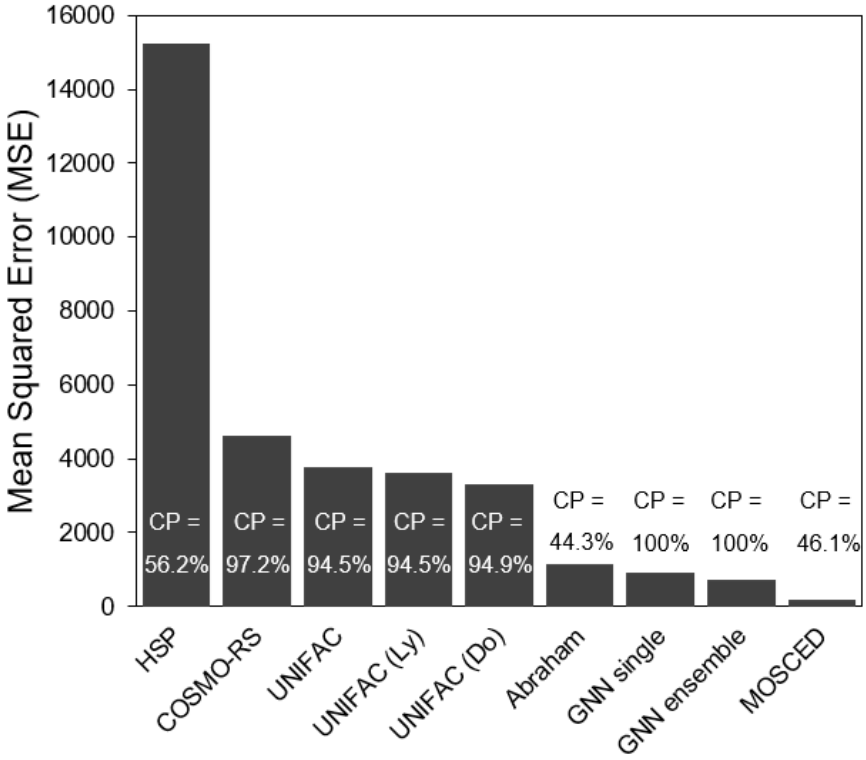


**Figure S3:** Comparison according to the Mean Squared Error (MSE). The performance reported for the GNN-based models corresponds to the test set.

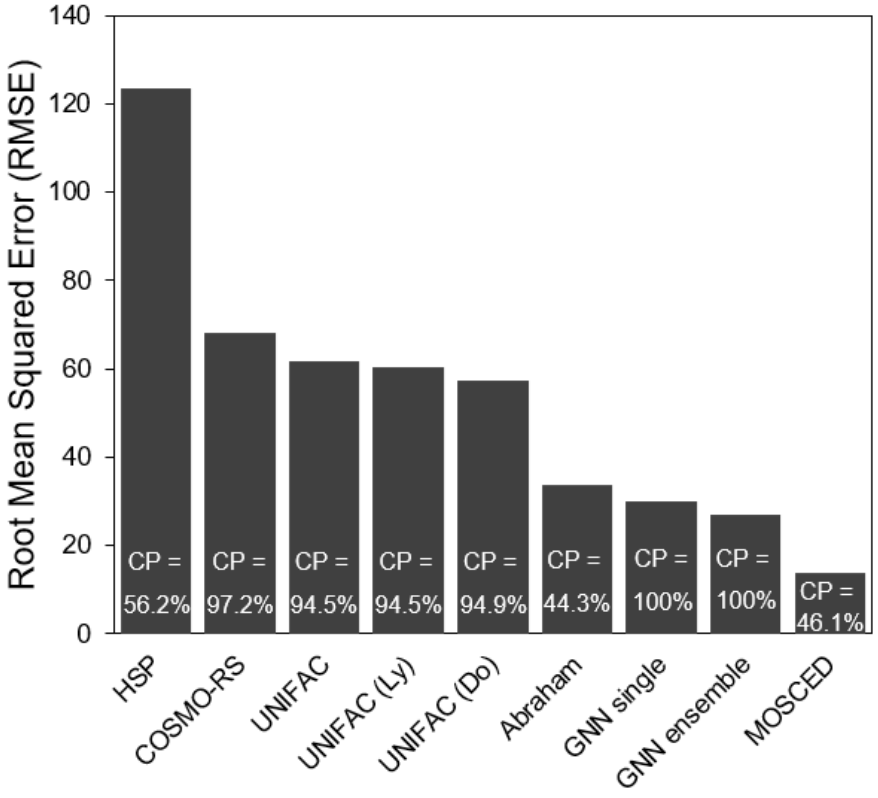


**Figure S4:** Comparison according to the Root Mean Squared Error (RMSE). The performance reported for the GNN-based models corresponds to the test set.

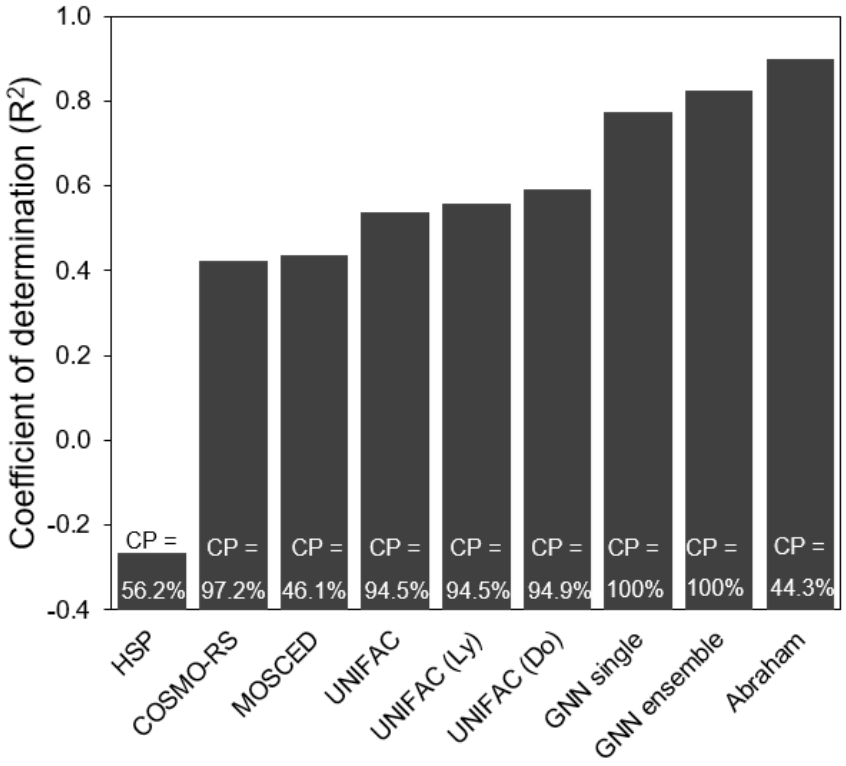


**Figure S5:** Comparison according to the coefficient of determination ($R^2$). The performance reported for the GNN-based models corresponds to the test set.

## S4.2 Parity plots comparing each mechanistic model to the corresponding GNN ensemble model

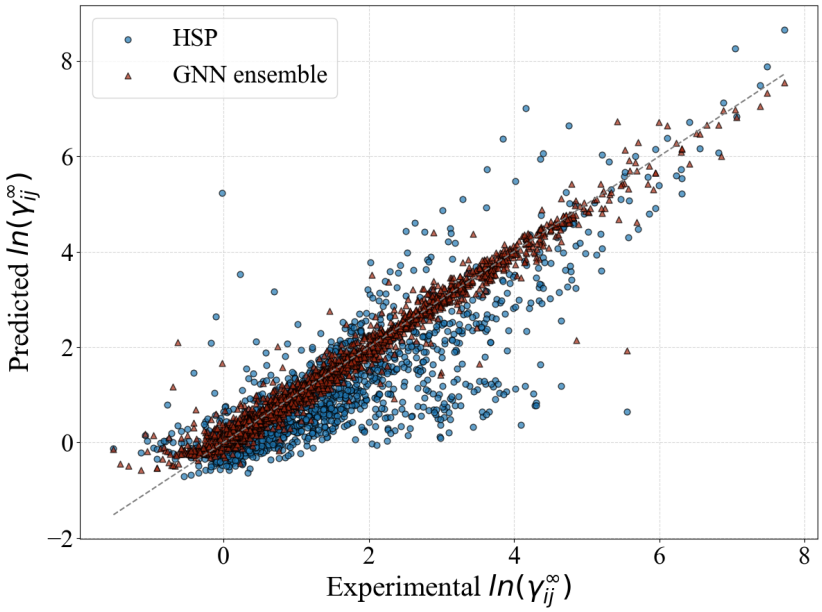


**Figure S6:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to HSP. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

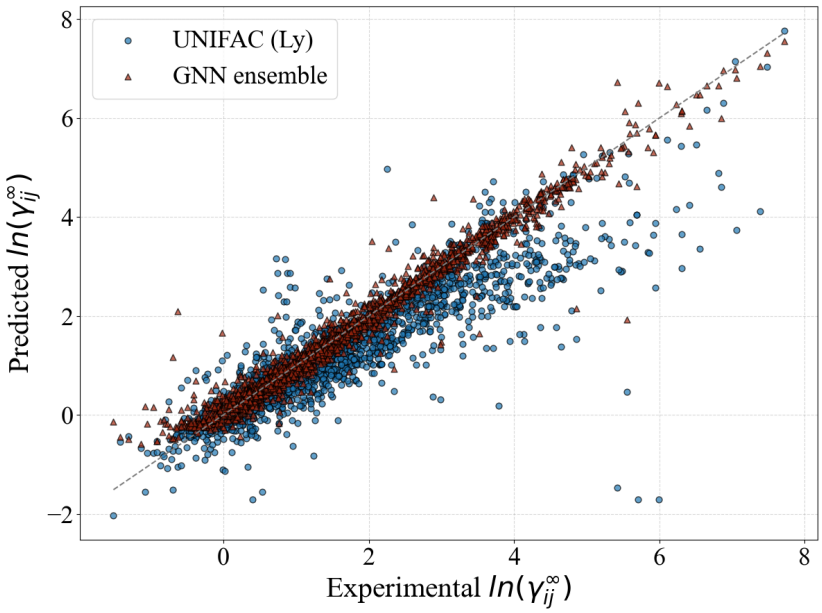


**Figure S7:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to UNIFAC-Lyngby. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

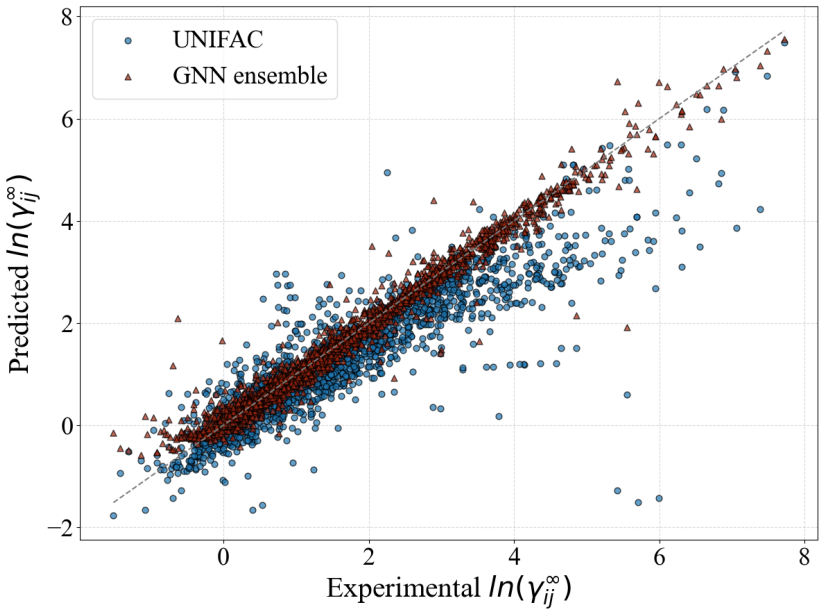


**Figure S8:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to UNIFAC. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

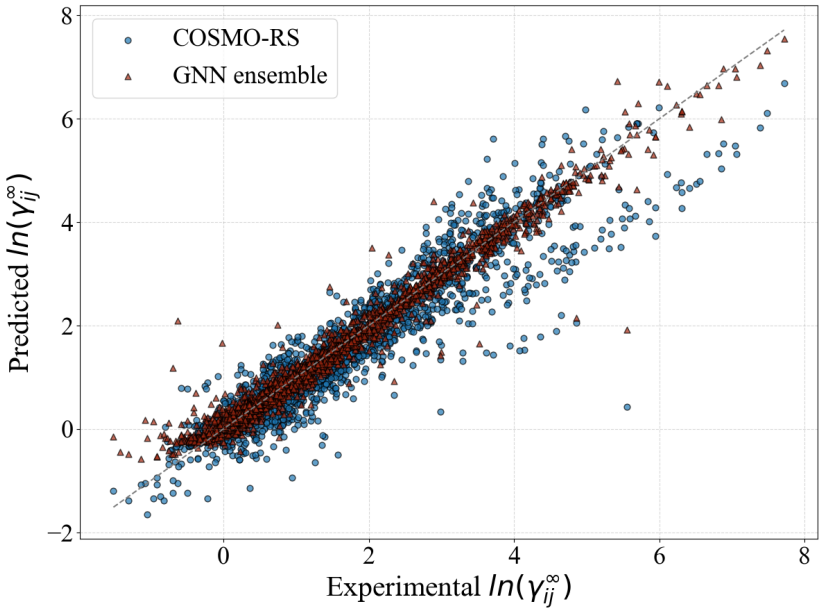


**Figure S9:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to COSMO-RS. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

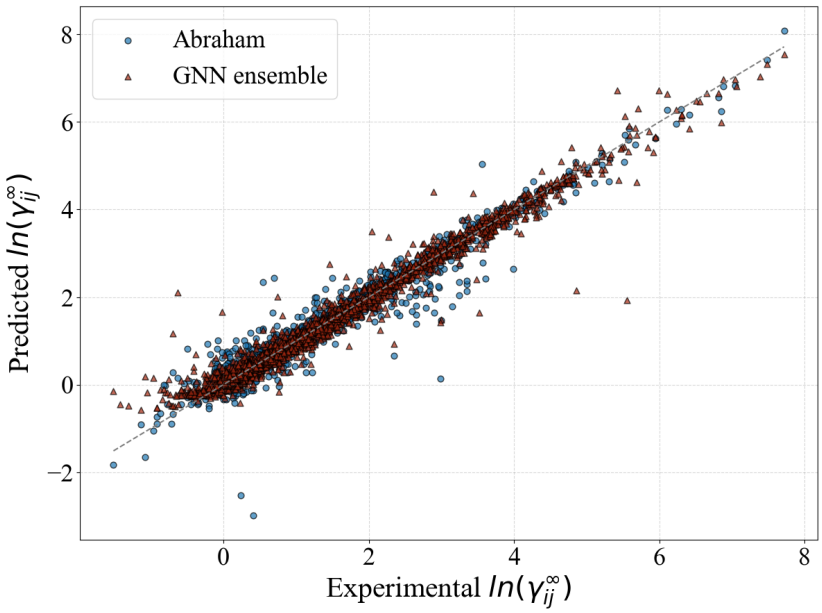


**Figure S10:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to Abraham. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

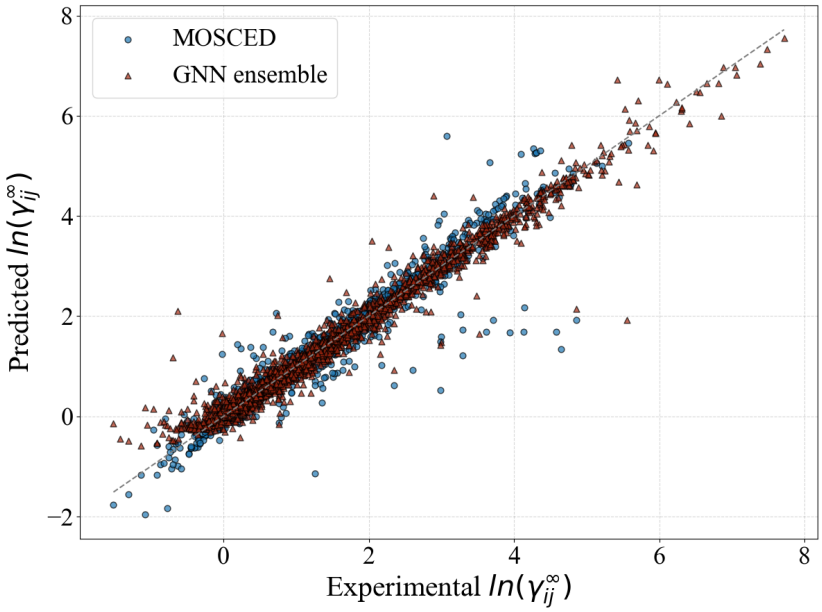


**Figure S11:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to MOSCED. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

## S4.3 Parity plots comparing each mechanistic model to the corresponding GNN ensemble model and hybrid GNN model

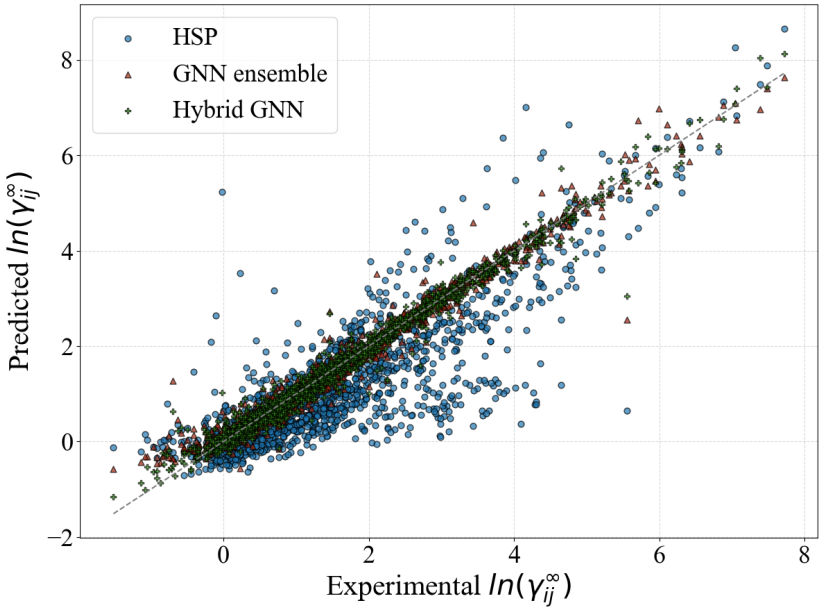


**Figure S12:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to HSP. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

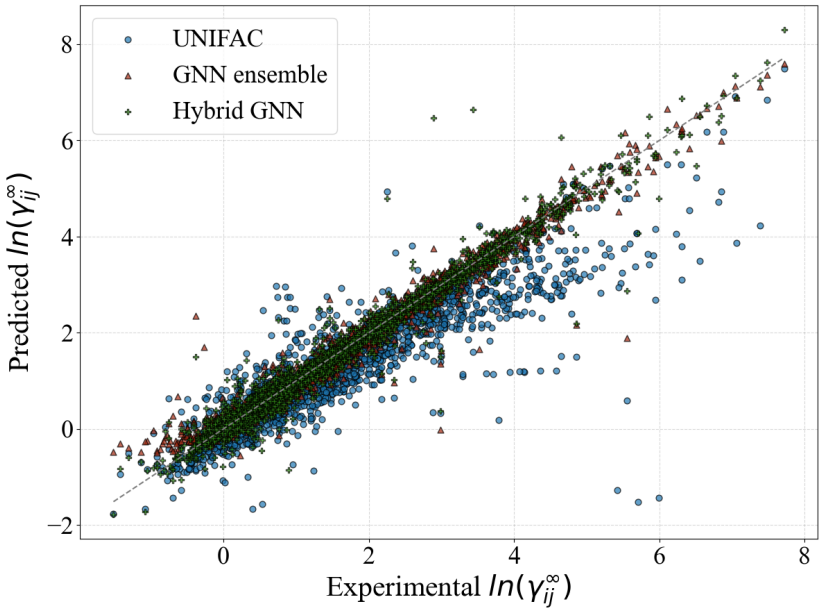


**Figure S13:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

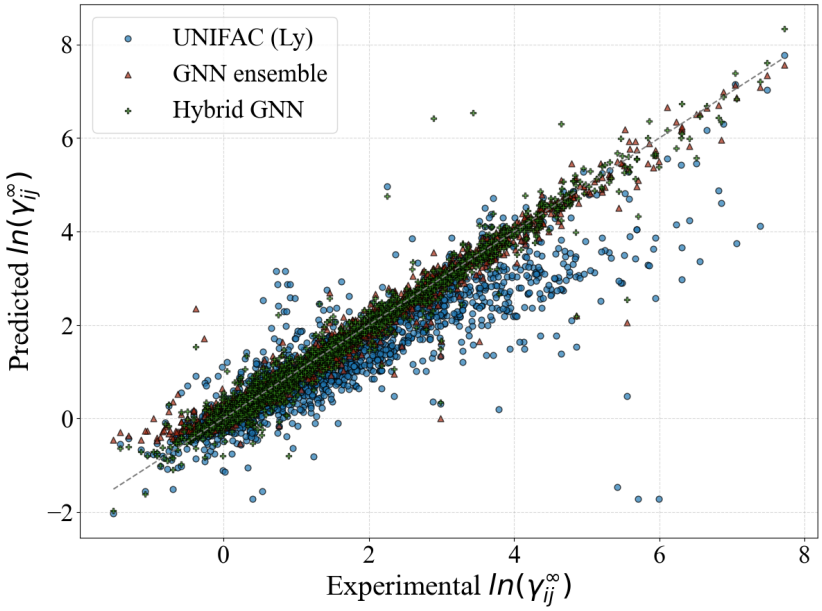


**Figure S14:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC-Lyngby. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

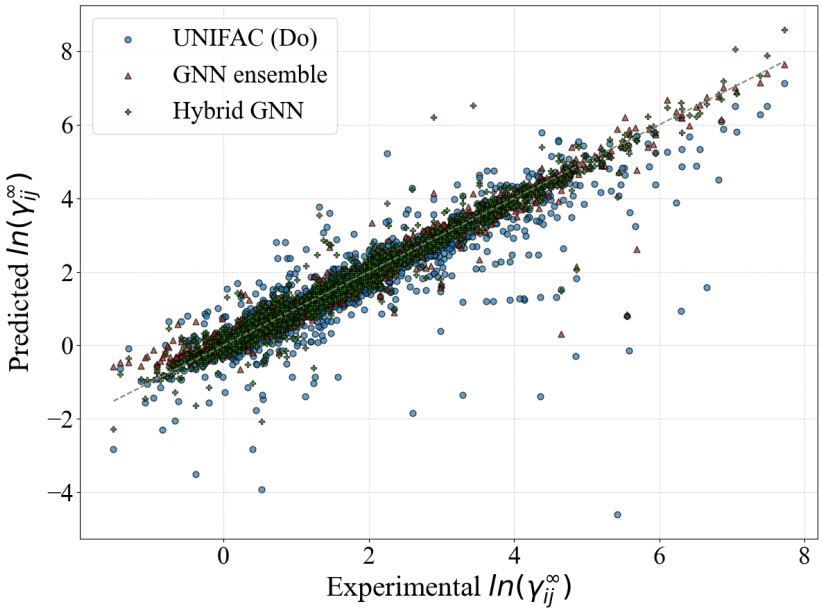


**Figure S15:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC-Dortmund. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

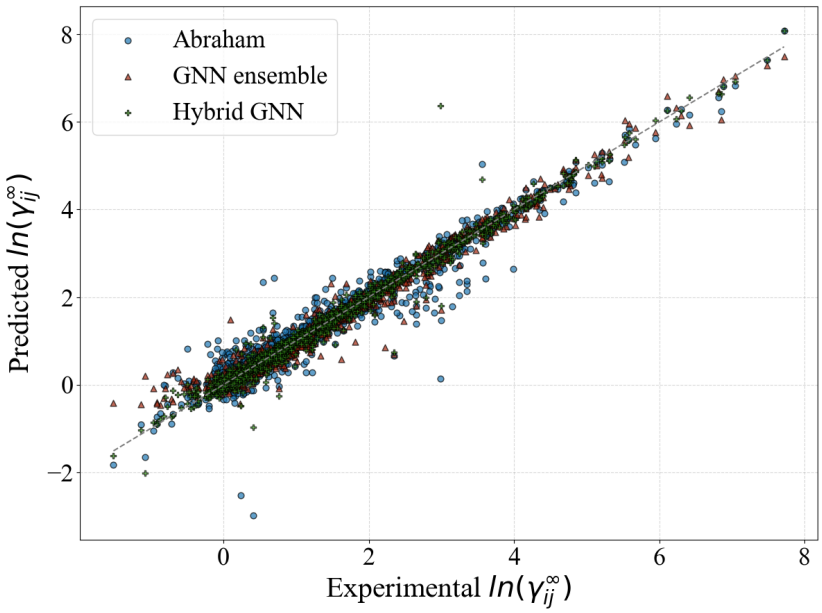


**Figure S16:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to Abraham. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

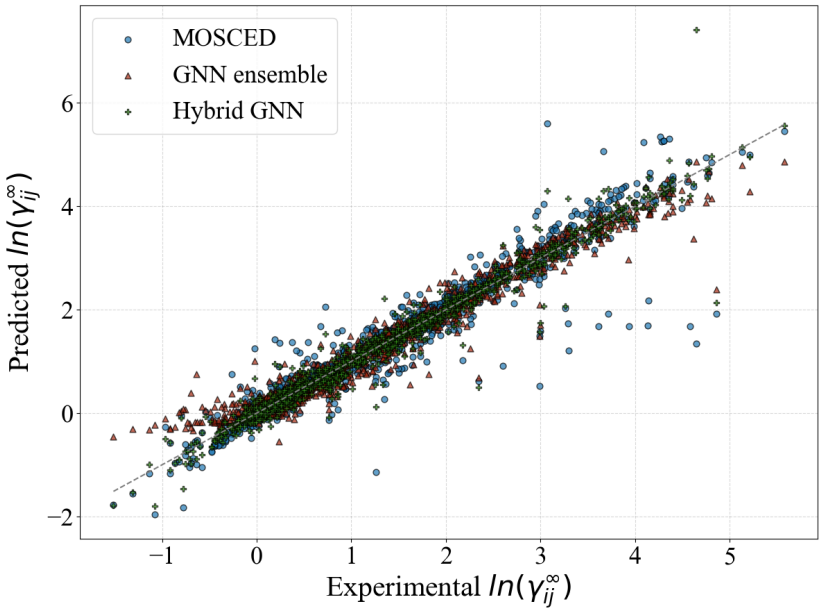


**Figure S17:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to MOSCED. The gray line corresponds to the perfect prediction. All the systems covered by each method are included in the plot.

## S4.4 Comparison of models on the feasible systems in the test set

The table and plots contained in this subsection show exclusively the comparison between the different models on the corresponding feasible systems contained in the test set. All the scores were calculated using the actual unscaled $\gamma_{i,j}^{\infty}$ values.

**Table S4:** Comparison of the performance between the GNN ensemble and the main 7 mechanistic models using only the feasible molecules of the corresponding method contained in the test dataset (percentage of this overlap is shown in the table). Note that for $R^2$ high values are desired while for the other metrics low indicates a better performance. For each pair the best scores are shown as bold numbers.

| Model | Overlap | MAE | SDEP | MSE | RMSE | $R^2$ | MAPE |
|---|---|---|---|---|---|---|---|
| HSP | 56.23% | 10.38 | 35.47 | 1365.99 | 3.22 | 0.69 | 114 |
| GNN HSP | - | **3.77** | **17.42** | **317.84** | **1.94** | **0.93** | **28** |
| UNIFAC (Ly) | 94.13% | 9.95 | 57.24 | 3375.3 | 3.15 | 0.23 | 30 |
| GNN UNIFAC (Ly) | - | **4.05** | **27.54** | **774.6** | **2.01** | **0.82** | **23** |
| UNIFAC | 94.13% | 9.8 | 55.81 | 3210.33 | 3.13 | 0.27 | 29 |
| GNN UNIFAC | - | **4.05** | **27.54** | **774.6** | **2.01** | **0.82** | **23** |
| COSMO-RS | 97.15% | 8.88 | 52.18 | 2801.78 | 2.98 | 0.34 | 27 |
| GNN COSMO-RS | - | **4.0** | **27.11** | **750.96** | **2.0** | **0.82** | **23** |
| UNIFAC (Do) | 94.66% | 7.12 | 43.48 | 1941.19 | 2.67 | 0.54 | 25 |
| GNN UNIFAC (Do) | - | **3.6** | **25.39** | **657.84** | **1.9** | **0.84** | **23** |
| Abraham | 44.66% | **4.05** | **28.65** | **836.99** | **2.01** | **0.85** | **23** |
| GNN Abraham | - | 4.94 | 35.87 | 1311.0 | 2.22 | 0.76 | 28 |
| MOSCED | 44.66% | 3.52 | 14.93 | 235.2 | 1.88 | 0.2 | **23** |
| GNN MOSCED | - | **1.68** | **5.26** | **30.47** | **1.3** | **0.9** | 28 |

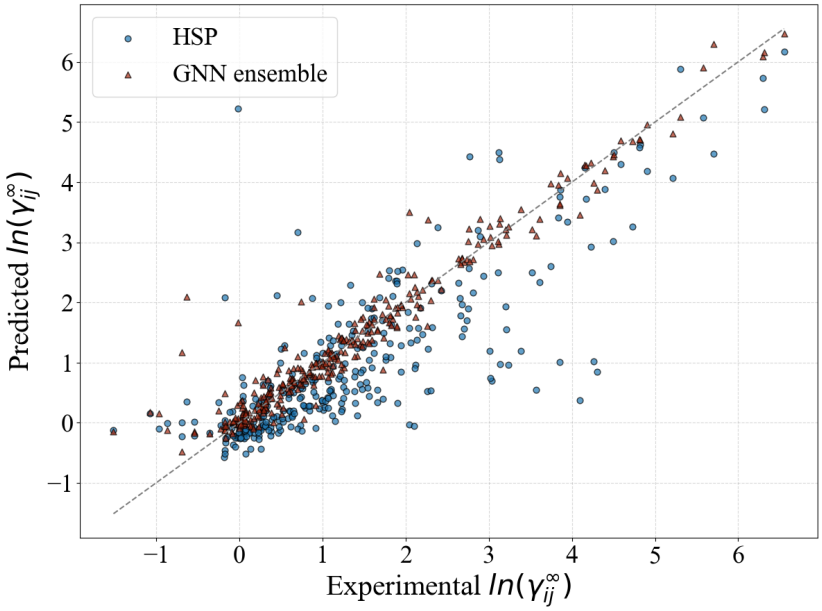


**Figure S18:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to HSP. Only the feasible molecules for HSP in the test set are shown. The gray line corresponds to the perfect prediction.

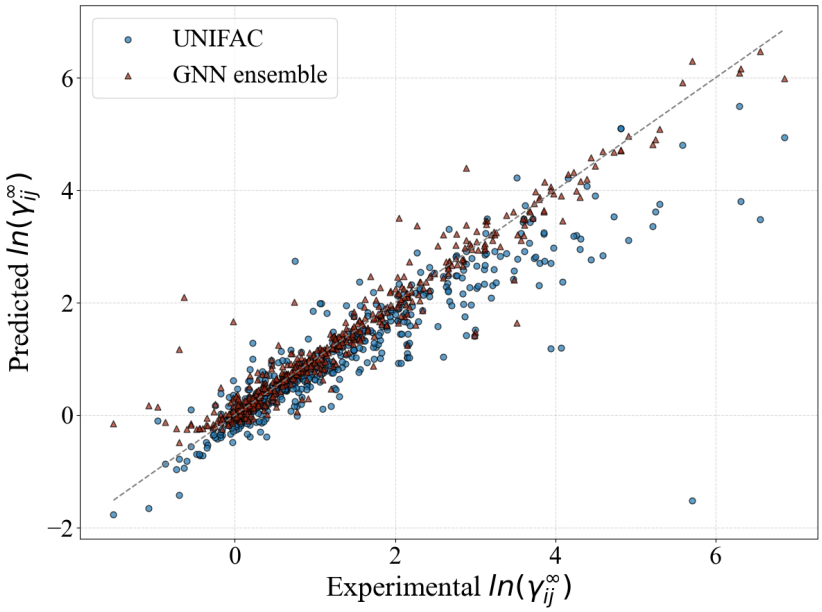


**Figure S19:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to UNIFAC. Only the feasible molecules for UNIFAC in the test set are shown. The gray line corresponds to the perfect prediction.

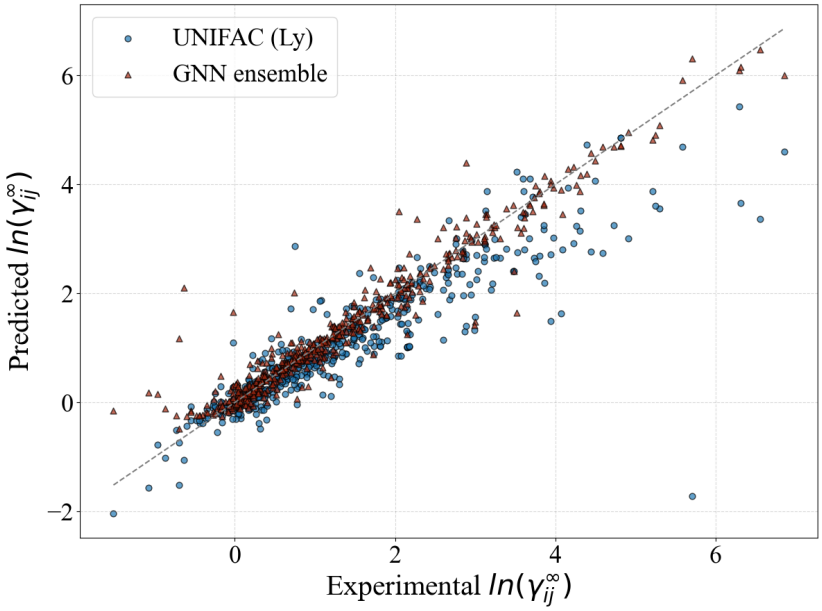


**Figure S20:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to UNIFAC-Lyngby. Only the feasible molecules for UNIFAC-Lyngby in the test set are shown. The gray line corresponds to the perfect prediction.

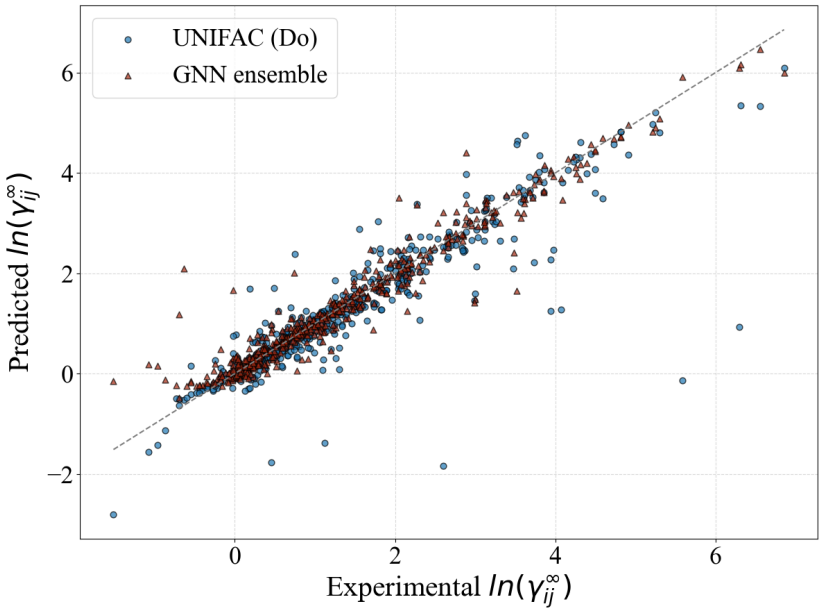


**Figure S21:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to UNIFAC-Dortmund. Only the feasible molecules for UNIFAC-Dortmund in the test set are shown. The gray line corresponds to the perfect prediction.

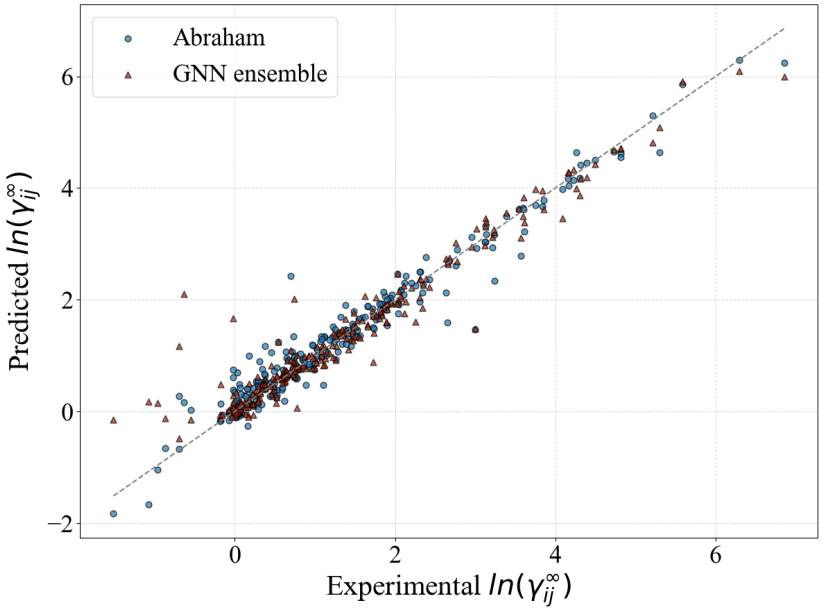


**Figure S22:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to Abraham. Only the feasible molecules for Abraham in the test set are shown. The gray line corresponds to the perfect prediction.

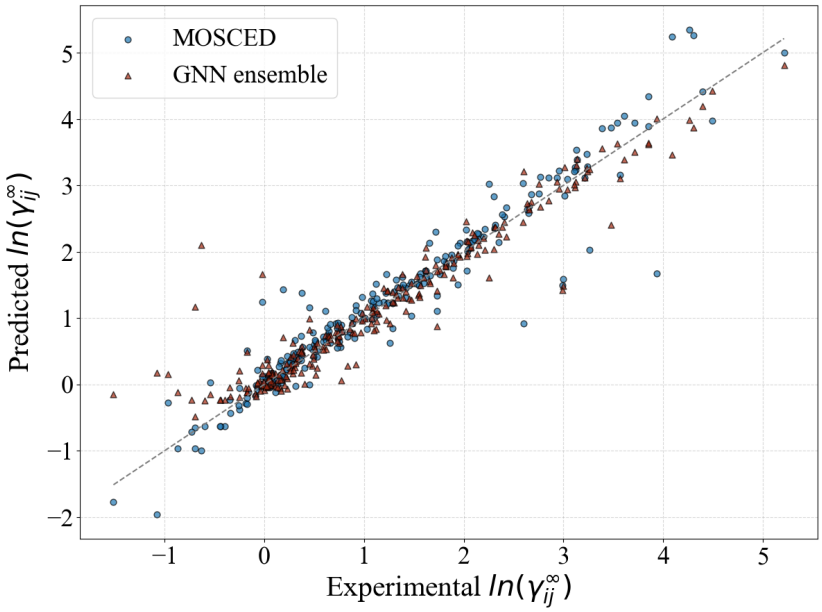


**Figure S23:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to MOSCED. Only the feasible molecules for MOSCED in the test set are shown. The gray line corresponds to the perfect prediction.

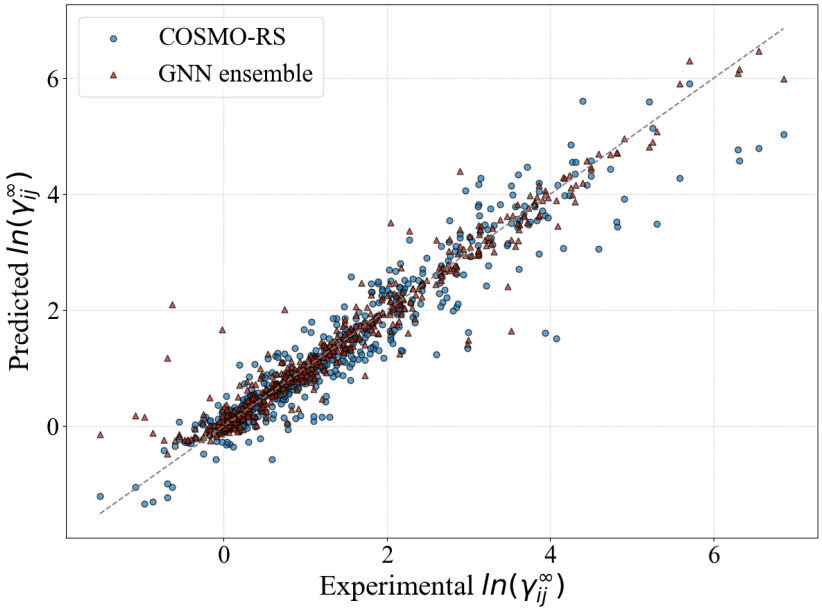


**Figure S24:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method, and the comparison to COSMO-RS. Only the feasible molecules for COSMO-RS in the test set are shown. The gray line corresponds to the perfect prediction.

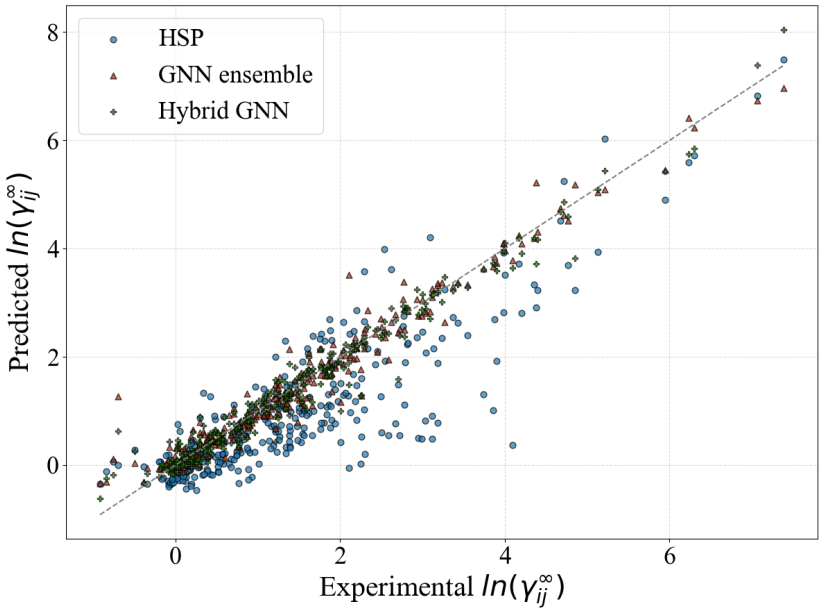


**Figure S25:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to HSP. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

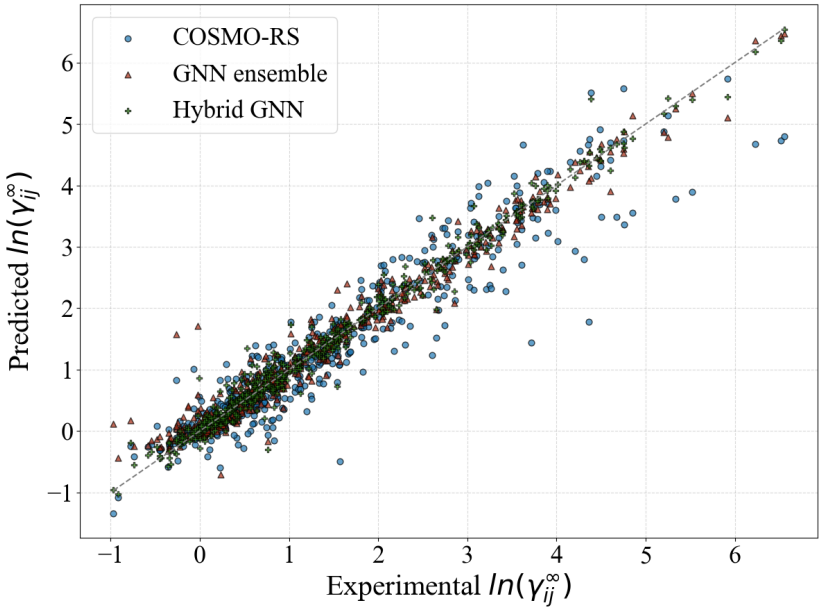


**Figure S26:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to COSMO-RS. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

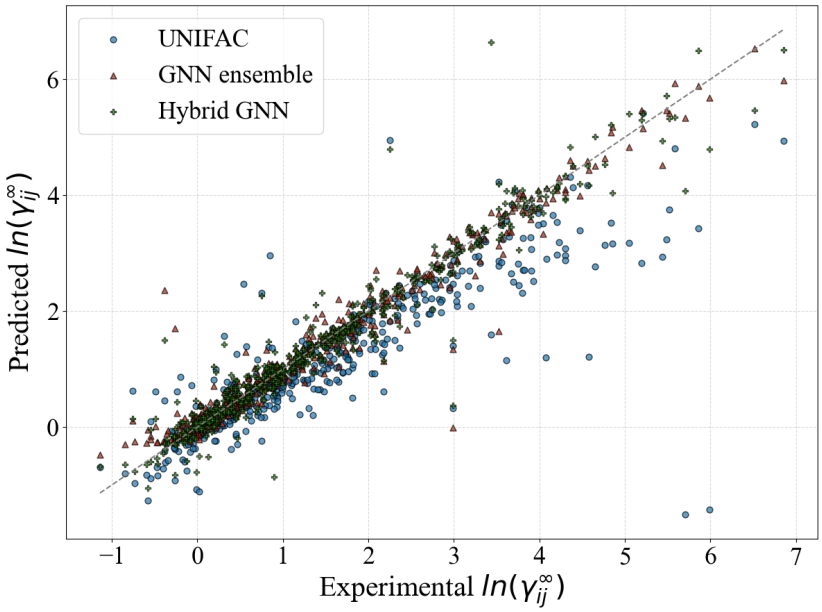


**Figure S27:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

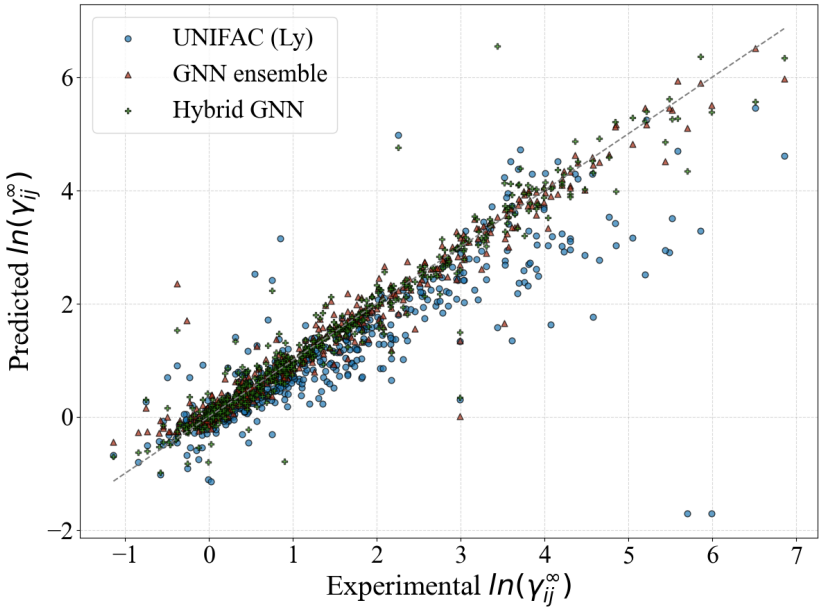


**Figure S28:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC-Lyngby. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

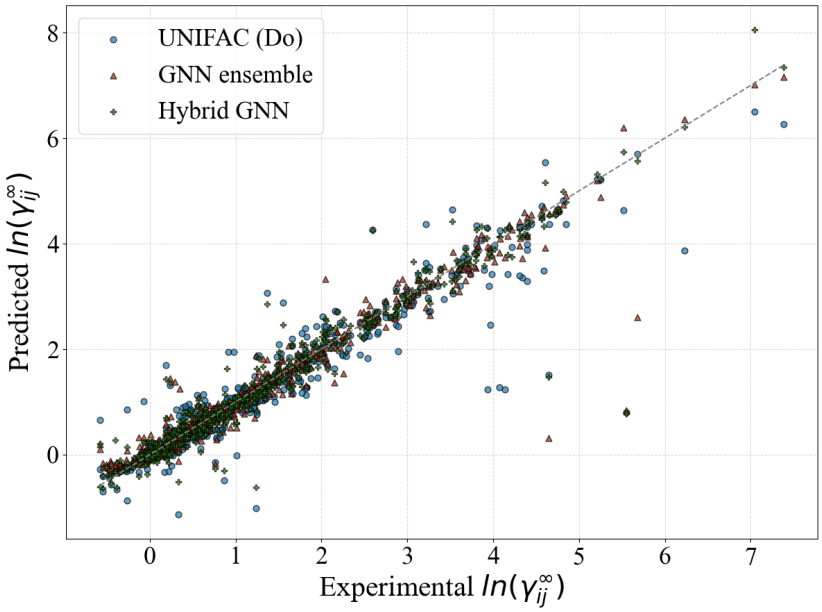


**Figure S29:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to UNIFAC-Dortmund. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

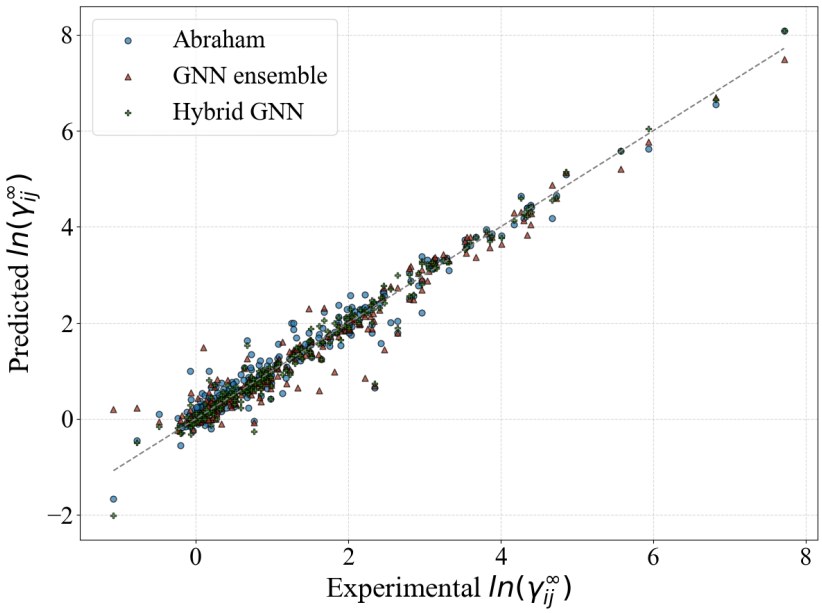


**Figure S30:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to Abraham. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

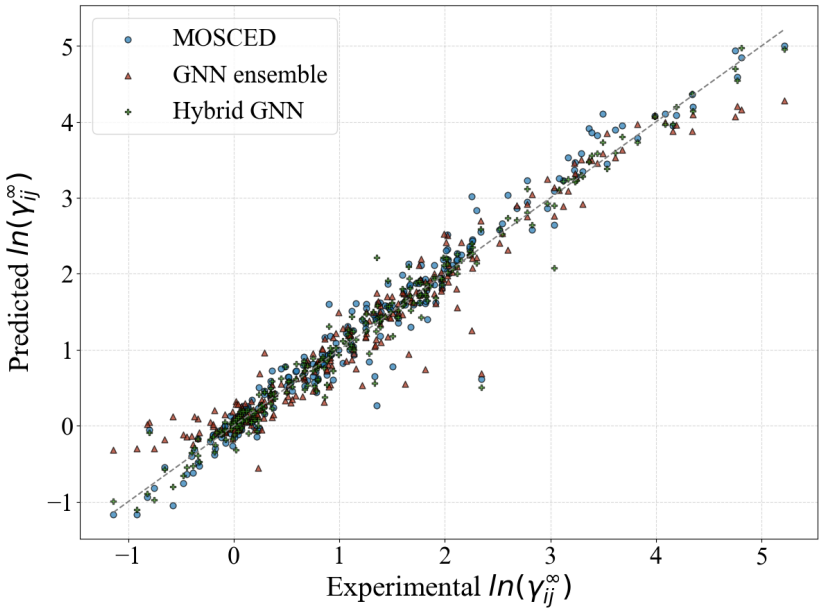


**Figure S31:** Parity plot of the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ with the proposed GNN ensemble method and hybrid GNN, and the comparison to MOSCED. The results are shown only for the systems defining the test set. The gray line corresponds to the perfect prediction.

## S4.5 Comparison of models considering the complete dataset and test dataset

The plots contained in this subsection show a comparison between the predictions of the corresponding GNN-based models on the test set and the predictions of the corresponding mechanistic models in the complete dataset. All the scores were calculated using the actual unscaled $\gamma_{i,j}^{\infty}$ values. These results enlarged the discussion contained in Section 3.2 of the main manuscript.

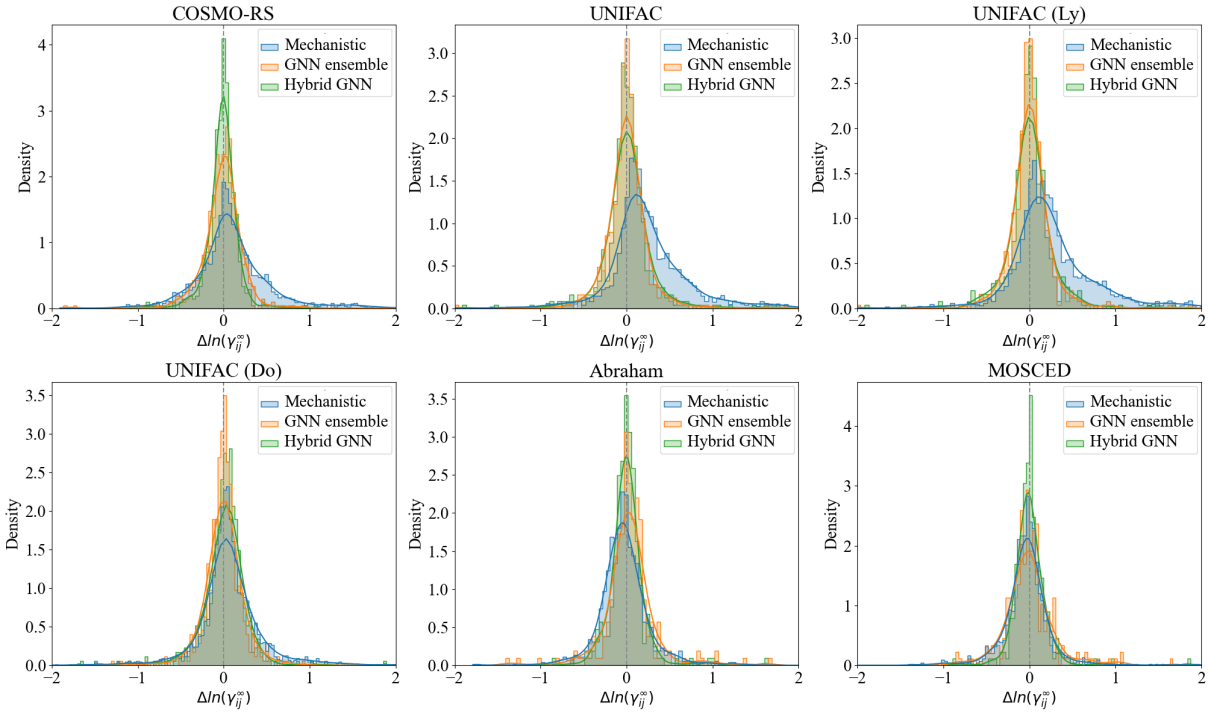


**Figure S32:** Density plots of the performance of the corresponding mechanistic models, the GNN ensemble and the hybrid GNN-based model. $\Delta ln(\gamma_{ij}^{\infty}) = ln(\gamma_{ij}^{\infty})^{exp} - ln(\gamma_{ij}^{\infty})^{pred}$, with (exp) being the experimental values gathered from the literature, and (pred) represents the predicted values by the corresponding method. Only errors in the range (-2,2) are shown. The gray central line shows the null-error for comparison. The results are shown for the test set for both GNN-based models, and for the complete dataset for the Mechanistic models.

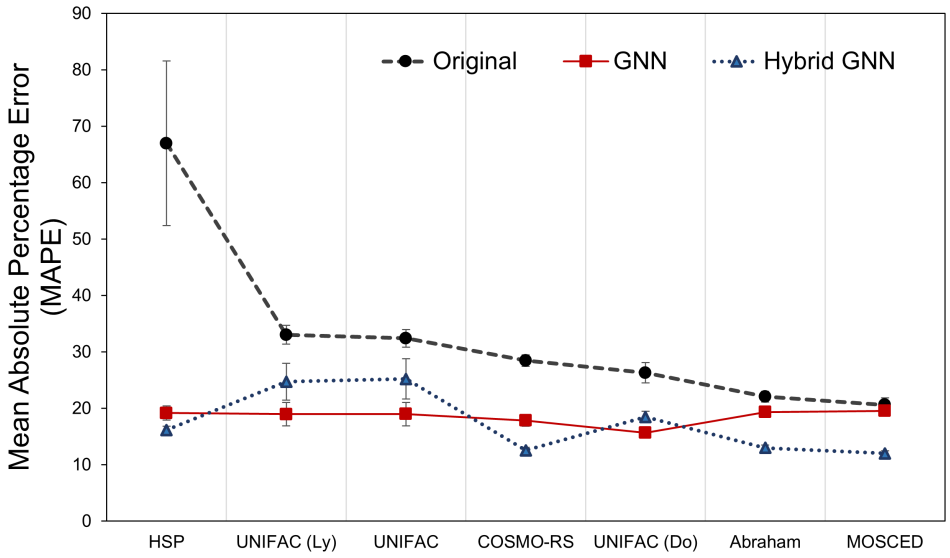


**Figure S33:** Mean absolute percentage error (MAPE) for the prediction of $\gamma_{ij}^{\infty}$ using the original mechanistic methods and the proposed GNN ensemble model and GNN-based hybrid model. Lower is better. Error bars show 3 times the standard deviation of the means. The results are shown for the test dataset in the case of GNN-ensemble and Hybrid GNN, and for the complete dataset for the Original models.

## S4.6 Ensemble size analysis

The size of the ensemble used in this work was determined by analyzing the performance of consecutive inclusions of GNN models into an ensemble according to their performance in the train/validation set. Figure S34 shows the decrements of the MAPE as more models are included into the ensemble. After around 20 models the MAPE starts to stabilize. 30 models were included to ensure the robustness of the predictions and to increase the significance of the provided error bars.

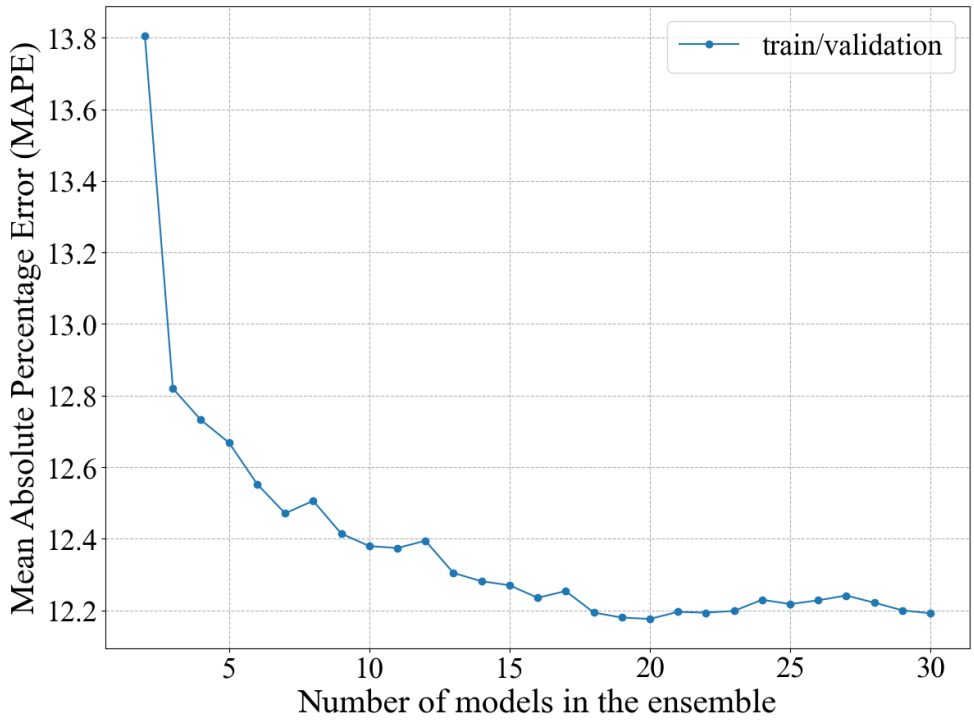


**Figure S34:** Comparison of the performance of GNN ensembles of different sizes on the train/validation set. Notice that after around 20 models the MAPE starts to stabilize. 30 models were included to ensure the robustness of the predictions and to increase the significance of the provided error bars.

## S4.7 Robustness analysis using 5-fold cross-validation

The table and the plots in this subsection show exclusively the comparison between the different models on the corresponding feasible systems contained in the test set averaged across the 5-folds used for cross-validation. Therefore, at each fold 20% of the data was reserved for testing while the rest was used for training a single GNN. In this way, the robustness of the predictions is examined with respect to their sensitivity to the random split taken. All the scores were calculated using the actual unscaled $\gamma_{i,j}^{\infty}$ values. The following conclusions can be drawn:

- The GNN model achieves better performance scores (according to their mean value) for all metrics compared to all mechanistic models. The only exception to this is when compared to the Abraham model, which achieves best performance than the GNN according to the mean values of the following metrics: MAE, SDEP, RMSE and $R^2$.
- The GNN model achieves lower standard deviation values compared to most mechanistic models for the following metrics: MAE, SDEP and MSE. However, the mechanistic models achieve lower standard deviation values in most comparisons on the following metrics: RMSE, $R^2$ and MAPE. While smaller standard deviation values correlates with a better robustness of the model, the mean values have to be also considered when assessing the type of robustness that the user of the model looks for. For instance, when looking at Figure S35, even though the spread of the GNN predictions is higher than the mechanistic ones, the predicted values remained better overall. The exception to this is the two specialized Abraham and MOSCED models.
- The overlap percentages are very similar to the percentage of systems covered (cf. Table 3 in the manuscript) and the overlap for the reported test set (cf. Table S4 in this ESI). This shows that the test set used for reporting the performance of the GNN model is indeed representative of the complete dataset.
- Overall, the GNN model presents better or on-pair robustness performance than most of the mechanistic models and for the systems analyzed in this work. However, this trend is not observable in the comparisons to the Abraham and MOSCED models, which have the smallest coverage of systems among all (cf. Table 3 in the manuscript).

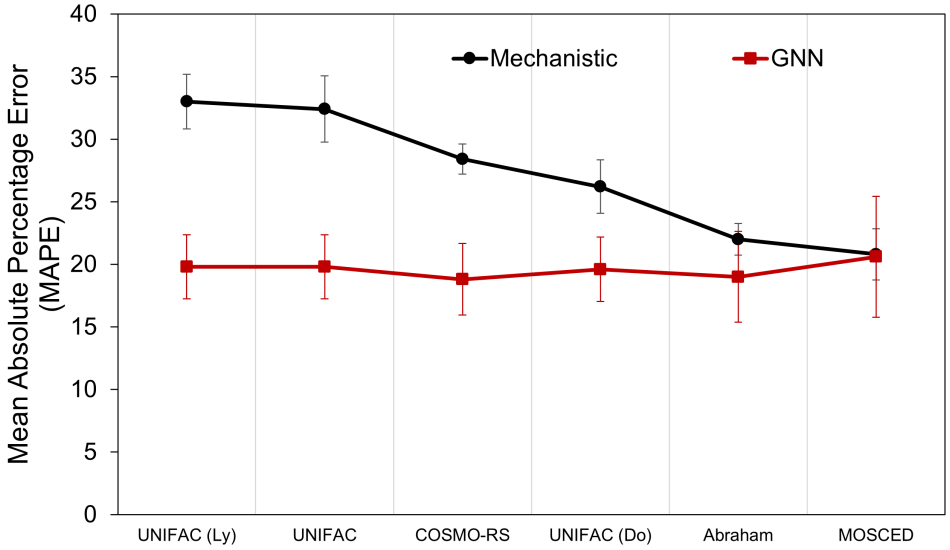


**Figure S35:** Mean absolute percentage error (MAPE) for the prediction of $\gamma_{ij}^{\infty}$ using the best mechanistic methods and the proposed GNN model. Lower is better. Error bars show one standard deviation from the means. The results are shown only for feasible systems contained in the test set in a 5-fold cross validation.

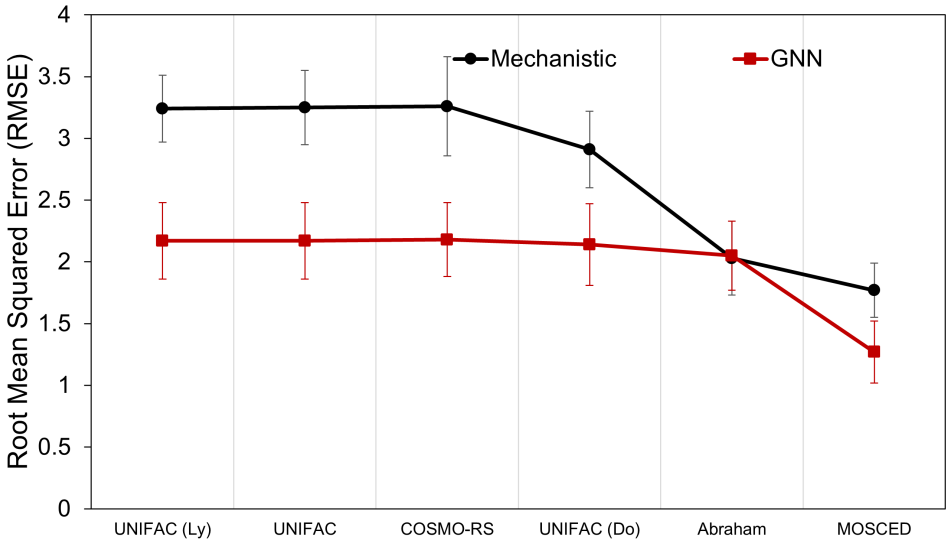


**Figure S36:** Root mean squared error (RMSE) for the prediction of $\gamma_{ij}^{\infty}$ using the best mechanistic methods and the proposed GNN model. Lower is better. Error bars show one standard deviation from the means. The results are shown only for feasible systems contained in the test set in a 5-fold cross validation.

**Table S5:** Results obtained from a 5-fold cross-validation. The performance metrics were calculated using only the feasible systems contained in the test set of each fold. Results are averaged across all the 5-folds and the standard deviation is shown next to the mean. The metrics were calculated using the unscaled $\gamma_{ij}^{\infty}$ values. Note that for $R^2$ high values are desired while for the other metrics low indicates a better performance. For each pair the best scores (according to their mean value) are shown as bold numbers. Moreover, for each pair the smallest standard deviation value is marked with an asterisk.

| Metric | Method | HSP | UNIFAC (Ly) | UNIFAC | COSMO-RS | UNIFAC (Do) | Abraham | MOSCED |
|---|---|---|---|---|---|---|---|---|
| Overlap | GNN | 56.23% | 94.52% | 94.52% | 97.22% | 94.91% | 44.27% | 46.12% |
| MAE | GNN | **5.05 ± 1.19*** | **4.82 ± 1.47*** | **4.82 ± 1.47*** | **4.82 ± 1.42*** | **4.69 ± 1.56*** | 4.3 ± 1.22 | **1.69 ± 0.72*** |
| | Mechanistic | 16.02 ± 5.54 | 10.59 ± 1.69 | 10.67 ± 1.87 | 10.8 ± 2.56 | 8.54 ± 1.73 | **4.2 ± 1.19*** | 3.17 ± 0.79 |
| SDEP | GNN | **27.72 ± 11.96*** | **32.96 ± 17.66*** | **32.96 ± 17.66*** | **32.58 ± 17.43*** | **32.27 ± 18.07*** | 28.29 ± 8.55* | **5.18 ± 3.55*** |
| | Mechanistic | 102.79 ± 66.7 | 55.36 ± 20.61 | 56.48 ± 21.55 | 61.74 ± 26.62 | 53.31 ± 19.3 | **27.22 ± 19.68** | 12.87 ± 4.25 |
| MSE | GNN | **938.45 ± 731.88*** | **1423.53 ± 1504.69*** | **1423.53 ± 1504.69*** | **1390.34 ± 1458.4*** | **1392.55 ± 1516.4*** | **893.08 ± 469.83*** | **42.82 ± 56.43*** |
| | Mechanistic | 15302.74 ± 16066.24 | 3604.78 ± 2349.38 | 3771.59 ± 2507.13 | 4643.54 ± 3402.37 | 3290.68 ± 1981.12 | 1147.07 ± 1473.47 | 194.42 ± 124.88 |
| RMSE | GNN | **2.23 ± 0.27*** | **2.17 ± 0.31** | **2.17 ± 0.31** | **2.18 ± 0.3*** | **2.14 ± 0.33** | 2.05 ± 0.28* | **1.27 ± 0.25** |
| | Mechanistic | 3.94 ± 0.68 | 3.24 ± 0.27* | 3.25 ± 0.3* | 3.26 ± 0.4 | 2.91 ± 0.31* | **2.03 ± 0.3** | 1.77 ± 0.22* |
| $R^2$ | GNN | **0.83 ± 0.15*** | **0.71 ± 0.32** | **0.71 ± 0.32** | **0.71 ± 0.32** | **0.71 ± 0.32** | 0.81 ± 0.14 | **0.91 ± 0.07*** |
| | Mechanistic | -0.5 ± 1.2 | 0.47 ± 0.16* | 0.47 ± 0.13* | 0.4 ± 0.05* | 0.52 ± 0.11* | **0.91 ± 0.06*** | 0.44 ± 0.21 |
| MAPE | GNN | **21.6 ± 3.26*** | **19.8 ± 2.56** | **19.8 ± 2.56*** | **18.8 ± 2.86** | **19.6 ± 2.58** | **19.0 ± 3.63** | **20.6 ± 4.84** |
| | Mechanistic | 66.6 ± 23.89 | 33.0 ± 2.19* | 32.4 ± 2.65 | 28.4 ± 1.2* | 26.2 ± 2.14* | 22.0 ± 1.26* | 20.8 ± 2.04* |

## S5 Data set

The data is available from the literature and was collected in the work of Brouwer et al. [2] available online from https://pubs.acs.org/doi/10.1021/acs.iecr.9b00727. Here, we add the SMILES strings for the solvents and solutes. Whenever multiple sources were available for the same binary system, the arithmetic mean of all the values was reported and all the references from the individual values were also provided. Since we run our experiments using the scaled data with the natural logarithm, various instances were deleted from the original database whenever a prediction of $\gamma_{ij}^{\infty} = 0$ was encountered. This happens for the UNIFAC-Dortmund prediction of the following systems' ID: 135, 237, 2486, 2493, 2504, 2510, 2511, 2520, 2522 and 2525. As mentioned in the original work of Brouwer et al.[2] both analytical and non-analytical techniques were included into this database. Further permission related to the material contained in this database should be directed to the American Chemical Society indicating the original work by Brouwer et al.[2]. To facilitate comparison with the original database, the reference numbers provided here correspond to the reference numbers in the Supplementary Information of the original work by Brouwer et al.[2] also available in Section S6 of this supplementary material.



## References

[1] G. W. Bemis and M. A. Murcko, *Journal of Medicinal Chemistry*, 1996, **39**, 2887–2893.

[2] T. Brouwer and B. Schuur, *Industrial & Engineering Chemistry Research*, 2019, **58**, 8903–8914.

**Table S6:** Database for the predicted $ln\left(\gamma_{ij}^{\infty}\right)$ values by 8 mechanistic models, and the values reported from the literature obtained experimentally.

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | BrC(Br)C(Br)Br | CCCCCC | 2.25 | 3.67 | 3.50 | 1.25 | | 2.45 | 4.25 | | 2.37 | [47] |
| 1 | BrC(Br)C(Br)Br | C1CCCCC1 | 1.80 | 2.94 | 2.93 | 1.74 | | 1.26 | 2.64 | | 1.62 | [47] |
| 2 | BrC(Br)C(Br)Br | c1ccccc1 | -0.60 | 0.76 | 0.84 | -0.04 | | 0.46 | 1.47 | | 0.22 | [47] |
| 3 | BrC(Br)C(Br)Br | CC=C(C)C | 0.83 | 2.32 | 2.12 | 1.09 | | 1.74 | 4.15 | | 1.31 | [47] |
| 4 | BrC(Br)C(Br)Br | CC(=C)C=C | 0.24 | 0.46 | 0.41 | 1.05 | | | | | 0.90 | [47] |
| 5 | ClC(Cl)C(Cl)Cl | CCCCC | 0.76 | 0.92 | 0.92 | 1.14 | | 0.72 | 1.03 | | 1.16 | [47] |
| 6 | ClC(Cl)C(Cl)Cl | CCC(C)C | 0.73 | 0.91 | 0.92 | 1.14 | | 0.95 | 1.42 | | 1.53 | [47] |
| 7 | ClC(Cl)C(Cl)Cl | CCCCCC | 0.84 | 1.09 | 1.08 | 1.26 | | 0.77 | 0.88 | | 1.27 | [47 , 48] |
| 8 | ClC(Cl)C(Cl)Cl | C1CCCCC1 | 0.64 | 0.97 | 0.90 | 1.15 | | 0.25 | 0.20 | | 1.03 | [47 , 49] |

Continued on next page

**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | ClC(Cl)C(Cl)Cl | c1ccccc1 | 0.16 | -0.42 | -0.54 | -0.29 | | -0.04 | -0.17 | | -0.22 | [47] |
| 10 | ClC(Cl)C(Cl)Cl | CC=C(C)C | 0.34 | 0.67 | 0.68 | 0.77 | | 0.41 | 0.81 | | 0.59 | [47] |
| 11 | ClC(Cl)C(Cl)Cl | CC(=C)C=C | 0.22 | 0.29 | 0.31 | 0.31 | | | | | 0.34 | [47] |
| 12 | ClC(Cl)C(Cl)Cl | CC(C)=O | -1.66 | -0.84 | -0.78 | -1.05 | | 0.03 | -0.30 | | -1.05 | [50] |
| 13 | N#CCCCCCCCCCCCCC#N | c1ccccc1 | | -0.40 | -0.21 | -0.15 | | | | | 0.10 | [51] |
| 14 | N#CCCCCCCCCCCCCC#N | Cc1ccccc1 | | -0.13 | 0.00 | -0.04 | | | | | 0.10 | [51] |
| 15 | N#CCCCCCCCCCCCCC#N | CCc1ccccc1 | | 0.07 | 0.14 | 0.30 | | | | | 0.41 | [51] |
| 16 | BrCCBr | c1ccccc1 | -0.46 | -0.02 | -0.11 | 0.05 | | 0.14 | 0.00 | | 0.50 | [52 , 53] |
| 17 | BrCCBr | Cc1ccccc1 | -0.27 | 1.24 | 1.15 | -0.13 | | 0.14 | 0.10 | | 0.49 | [53] |
| 18 | ClCCCl | CCCCC | 1.34 | 0.95 | 0.92 | 1.14 | 1.44 | 0.95 | 1.15 | 1.53 | 1.50 | [54] |
| 19 | ClCCCl | CCCCCC | 1.49 | 1.09 | 1.08 | 1.26 | 1.57 | 1.00 | 1.01 | 1.58 | 1.50 | [54 , 55 , 56] |
| 20 | ClCCCl | C1CCCCC1 | 1.27 | 0.91 | 0.90 | 1.15 | 1.16 | 0.46 | 0.39 | 1.24 | 1.42 | [54 , 56] |
| 21 | ClCCCl | CCCC(C)C | 1.44 | 1.09 | 1.07 | 1.26 | 1.59 | | | 1.70 | 1.63 | [54] |
| 22 | ClCCCl | CCCCCCC | 1.64 | 1.21 | 1.21 | 1.39 | 1.69 | 1.04 | 0.88 | 1.66 | 1.76 | [54] |
| 23 | ClCCCl | CC(C)CC(C)C | 1.53 | 1.21 | 1.21 | 1.39 | 1.70 | | | 1.88 | 1.73 | [54] |
| 24 | ClCCCl | CCCCCCCC | 1.78 | 1.32 | 1.35 | 1.51 | 1.85 | 1.12 | 0.82 | 1.74 | 1.86 | [54] |
| 25 | ClCCCl | CC(C)C(C)C(C)C | 1.58 | 1.32 | 1.35 | 1.51 | 1.55 | | | | 1.72 | [54] |
| 26 | ClCCCl | CC(C)CCC(C)C | 1.69 | 1.32 | 1.35 | 1.51 | | | | | 1.82 | [54] |
| 27 | ClCCCl | CCC1CCCCC1 | 1.53 | 1.17 | 1.19 | 1.36 | | | | 1.53 | 1.60 | [54] |
| 28 | ClCCCl | CCCCCCCCC | 1.92 | 1.41 | 1.48 | 1.63 | 2.10 | 1.18 | 0.77 | 1.81 | 1.97 | [54] |
| 29 | ClCCCl | c1ccccc1 | 0.36 | -0.51 | -0.53 | -0.29 | 0.03 | 0.16 | 0.00 | 0.10 | 0.18 | [56] |
| 30 | N#CCCC#N | CCCCCC | 5.74 | 3.60 | 3.63 | 5.78 | | | | | 5.91 | [47] |
| 31 | N#CCCC#N | C1CCCCC1 | 4.90 | 3.09 | 3.06 | 5.53 | | | | | 4.88 | [47] |
| 32 | N#CCCC#N | c1ccccc1 | 2.37 | 1.15 | 1.04 | 1.95 | | | | | 2.03 | [47] |
| 33 | N#CCCC#N | CC=C(C)C | 3.78 | 2.70 | 2.69 | 4.34 | | | | | 3.81 | [47] |
| 34 | N#CCCC#N | CC(=C)C=C | 2.80 | 1.72 | 1.72 | 2.42 | | | | | 2.98 | [47] |
| 35 | CCOCCOCC | C1CCCCC1 | 0.53 | 0.51 | 0.46 | 0.32 | | | | | 0.67 | [57] |
| 36 | CCOCOCC | C1CCCCC1 | 0.53 | 0.67 | 0.60 | 0.43 | | | | | 0.46 | [57] |
| 37 | COCCOC | C1CCCCC1 | | 1.48 | 1.38 | 0.87 | | 0.32 | -0.16 | | 1.22 | [57] |
| 38 | ClCCCCl | CCCCCC | 1.38 | 1.04 | 1.05 | 1.54 | | 0.91 | 1.10 | | 0.79 | [55] |
| 39 | ClCCCCl | CC(C)=O | 0.49 | 0.01 | 0.01 | -0.29 | | 0.00 | -0.25 | | 0.07 | [55] |
| 40 | N#CCCCC#N | CCCCCC | 4.98 | 2.95 | 2.95 | 4.57 | | 3.15 | 4.95 | 4.38 | 4.62 | [47] |
| 41 | N#CCCCC#N | C1CCCCC1 | 4.23 | 2.51 | 2.48 | 4.30 | | 2.35 | 3.38 | 3.76 | 3.93 | [47] |
| 42 | N#CCCCC#N | c1ccccc1 | 1.87 | 0.81 | 0.73 | 1.37 | | 1.74 | 2.18 | 1.33 | 1.46 | [51 , 47] |
| 43 | N#CCCCC#N | Cc1ccccc1 | 2.45 | 1.16 | 1.05 | 1.71 | | 1.84 | 2.44 | 1.83 | 1.65 | [51] |
| 44 | N#CCCCC#N | CCc1ccccc1 | 3.01 | 1.60 | 1.49 | 2.57 | | 2.42 | 2.66 | 2.27 | 2.12 | [51] |
| 45 | N#CCCCC#N | CC=C(C)C | 3.21 | 2.16 | 2.14 | 3.38 | | 1.91 | 4.86 | | 3.21 | [47] |
| 46 | N#CCCCC#N | CC(=C)C=C | 2.37 | 1.31 | 1.32 | 1.75 | | | | | 2.39 | [47] |
| 47 | ClCCCCCl | CCCCCC | 1.26 | 2.46 | 2.46 | 3.77 | | 0.74 | 1.04 | | 1.31 | [55] |
| 48 | ClCCCCCl | CC(C)=O | -0.27 | 0.12 | 0.15 | -0.25 | | -0.07 | -0.31 | | 0.06 | [55] |
| 49 | N#CCCCCC#N | CCCCC | 3.58 | 2.10 | 2.11 | 3.42 | | 2.40 | 5.16 | | 3.55 | [58 , 47] |
| 50 | N#CCCCCC#N | C1CCCC1 | 3.00 | 1.70 | 1.70 | 2.90 | | 1.52 | 3.33 | | 2.74 | [58] |
| 51 | N#CCCCCC#N | CCC(C)C | 3.44 | 2.10 | 2.11 | 3.42 | | 2.62 | 5.98 | | 3.69 | [47] |
| 52 | N#CCCCCC#N | CCCCCC | 4.12 | 2.46 | 2.46 | 3.77 | | 2.70 | 4.80 | | 3.87 | [59 , 59 , 58 , 47 , 59 , 59] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 53 | N#CCCCCC#N | C1CCCCC1 | 3.47 | 2.08 | 2.06 | 3.50 | | 1.93 | 3.13 | | 3.20 | [58 , 47] |
| 54 | N#CCCCCC#N | CCCCCCC | 4.64 | 2.80 | 2.80 | 4.12 | | 2.99 | 4.46 | | 4.06 | [58] |
| 55 | N#CCCCCC#N | C1CCCCCC1 | 3.83 | 2.44 | 2.41 | 4.08 | | | | | 3.29 | [58] |
| 56 | N#CCCCCC#N | CCCCCCCC | 5.16 | 3.12 | 3.14 | 4.47 | | 3.31 | 4.29 | | 4.37 | [58] |
| 57 | N#CCCCCC#N | C1CCCCCCC1 | 4.15 | 2.78 | 2.75 | 4.64 | | 2.50 | 2.52 | | 3.52 | [58] |
| 58 | N#CCCCCC#N | CCCCCCCCC | 5.67 | 3.43 | 3.47 | 4.81 | | 3.62 | 4.13 | | 4.70 | [58] |
| 59 | N#CCCCCC#N | CCCCCCCCCC | 6.18 | 3.73 | 3.79 | 5.16 | | 3.97 | 4.15 | | 4.98 | [58] |
| 60 | N#CCCCCC#N | c1ccccc1 | 1.29 | 0.55 | 0.51 | 0.99 | | 1.35 | 1.88 | | 0.89 | [59 , 59 , 58 , 51 , 47 , 59 , 59] |
| 61 | N#CCCCCC#N | Cc1ccccc1 | 1.78 | 0.88 | 0.79 | 1.26 | | 1.43 | 2.15 | | 1.28 | [51] |
| 62 | N#CCCCCC#N | CCc1ccccc1 | 2.23 | 1.26 | 1.17 | 1.98 | | 1.95 | 2.38 | | 1.70 | [51] |
| 63 | N#CCCCCC#N | CC=C(C)C | 2.54 | 1.76 | 1.75 | 2.74 | | 1.53 | 4.70 | | 2.53 | [47] |
| 64 | N#CCCCCC#N | CC(=C)C=C | 1.78 | 1.00 | 1.03 | 1.32 | | | | | 1.73 | [47] |
| 65 | N#CCCCCC#N | CCCCC=C | 3.09 | 1.84 | 1.84 | 2.95 | | 2.36 | 4.95 | | 2.93 | [58] |
| 66 | N#CCCCCC#N | CCCCCC=C | 3.56 | 2.17 | 2.17 | 3.31 | | 2.33 | 4.48 | | 3.25 | [58] |
| 67 | N#CCCCCC#N | CCCCCCC=C | 4.14 | 2.49 | 2.50 | 3.67 | | 2.51 | 4.26 | | 3.58 | [58] |
| 68 | N#CCCCCC#N | CCCCC#C | 1.81 | 0.78 | 0.79 | 2.09 | | | | | 1.53 | [58] |
| 69 | N#CCCCCC#N | CCCCCC#C | 2.32 | 1.02 | 1.03 | 2.40 | | | | | 1.81 | [58] |
| 70 | N#CCCCCC#N | CCCCCCC#C | 2.80 | 1.24 | 1.28 | 2.72 | | | | | 2.16 | [58] |
| 71 | CN1CCN(C)CC1 | C1CCCCC1 | 0.29 | 0.11 | 0.12 | 0.39 | | | | | 0.25 | [60] |
| 72 | CN1CCN(C)CC1 | CCCCCCC | 0.41 | 0.22 | 0.18 | 0.10 | | | | | 0.35 | [60] |
| 73 | C1COCCO1 | CCCCC | 1.26 | 1.67 | 1.42 | 1.12 | 1.56 | 0.84 | 1.11 | 1.60 | 1.67 | [54 , 61 , 61] |
| 74 | C1COCCO1 | CCCCCC | 1.43 | 1.94 | 1.63 | 1.28 | 1.70 | 0.88 | 0.97 | 1.65 | 1.84 | [54 , 61 , 61] |
| 75 | C1COCCO1 | C1CCCCC1 | 1.22 | 1.92 | 1.38 | 1.09 | 1.39 | 0.34 | 0.33 | 1.23 | 1.53 | [54 , 61 , 61] |
| 76 | C1COCCO1 | CCCC(C)C | 1.37 | 1.94 | 1.63 | 1.28 | 1.72 | | | 1.79 | 1.82 | [54 , 61 , 61] |
| 77 | C1COCCO1 | CCCCCCC | 1.59 | 2.18 | 1.83 | 1.43 | 1.84 | 0.91 | 0.84 | 1.73 | 1.96 | [54 , 61 , 61] |
| 78 | C1COCCO1 | CC(C)CC(C)C | 1.46 | 2.19 | 1.83 | 1.43 | 1.84 | | | 1.99 | 1.97 | [54 , 61 , 61] |
| 79 | C1COCCO1 | CCCCCCCC | 1.74 | 2.42 | 2.03 | 1.57 | 2.03 | 0.97 | 0.78 | 1.81 | 2.12 | [54 , 61 , 61] |
| 80 | C1COCCO1 | CC(C)C(C)C(C)C | 1.50 | 2.42 | 2.02 | 1.57 | 1.72 | | | | 1.96 | [54 , 61 , 61] |
| 81 | C1COCCO1 | CC(C)CCC(C)C | 1.64 | 2.42 | 2.02 | 1.57 | | | | | 2.14 | [54] |
| 82 | C1COCCO1 | CCC1CCCCC1 | 1.50 | 2.44 | 1.79 | 1.33 | | | | 1.55 | 1.85 | [54 , 61 , 61] |
| 83 | C1COCCO1 | CCCCCCCCC | 1.89 | 2.63 | 2.22 | 1.71 | 2.29 | 1.03 | 0.72 | 1.88 | 2.29 | [54 , 61 , 61] |
| 84 | C1COCCO1 | CCC(C)CCC(C)C | 1.76 | 2.64 | 2.22 | 1.71 | | | | | 1.89 | [61] |
| 85 | C1COCCO1 | Cc1ccccc1 | 0.25 | 1.20 | 0.43 | -0.20 | 0.46 | 0.07 | 0.04 | 0.13 | 0.17 | [61] |
| 86 | C1COCCO1 | CCO | 0.80 | 0.82 | 0.83 | 0.76 | 1.15 | 0.52 | 0.94 | 1.00 | 0.91 | [61] |
| 87 | C1COCCO1 | CCC(C)=O | 0.17 | 0.49 | 0.31 | 0.03 | 0.47 | 0.32 | -0.11 | 0.22 | 0.22 | [61] |
| 88 | C1COCCO1 | CCN(CC)CC | 0.90 | 2.12 | 1.77 | 1.14 | 1.38 | 0.31 | 0.15 | 1.39 | 1.22 | [61] |
| 89 | N#CCCCCCC#N | CCCCCC | 3.43 | 2.09 | 2.09 | 3.20 | | | | | 3.42 | [47] |
| 90 | N#CCCCCCC#N | C1CCCCC1 | 2.88 | 1.74 | 1.75 | 2.93 | | | | | 2.84 | [47] |
| 91 | N#CCCCCCC#N | c1ccccc1 | 0.94 | 0.35 | 0.34 | 0.71 | | | | | 0.51 | [47] |
| 92 | N#CCCCCCC#N | CC=C(C)C | 2.06 | 1.45 | 1.45 | 2.28 | | | | | 2.16 | [47] |
| 93 | N#CCCCCCC#N | CC(=C)C=C | 1.41 | 0.76 | 0.82 | 1.03 | | | | | 1.39 | [47] |
| 94 | CC1CCC(=O)N1C | CCCCC | 1.44 | | | | | | | 1.96 | 1.94 | [62] |
| 95 | CC1CCC(=O)N1C | CCCCCC | 1.67 | | | | | | | 2.14 | 2.19 | [62] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 96 | CC1CCC(=O)N1C | C1CCCCC1 | 1.40 | | | | | | | 1.64 | 1.64 | [62] |
| 97 | CC1CCC(=O)N1C | CCCCCCC | 1.89 | | | | | | | 2.34 | 2.24 | [62] |
| 98 | CC1CCC(=O)N1C | CCCCCCCC | 2.11 | | | | | | | 2.53 | 2.41 | [62] |
| 99 | CC1CCC(=O)N1C | c1ccccc1 | 0.08 | | | | | | | -0.07 | -0.12 | [62] |
| 100 | CC1CCC(=O)N1C | Cc1ccccc1 | 0.33 | | | | | | | 0.14 | 0.10 | [62] |
| 101 | CC1CCC(=O)N1C | CCCC=C | 0.85 | | | | | | | 1.41 | 1.40 | [62] |
| 102 | CC1CCC(=O)N1C | CCCCC=C | 1.08 | | | | | | | 1.67 | 1.56 | [62] |
| 103 | CC1CCC(=O)N1C | C1CCC=CC1 | 0.88 | | | | | | | | 1.12 | [62] |
| 104 | CC1CCC(=O)N1C | CCCCCC=C | 1.28 | | | | | | | | 1.67 | [62] |
| 105 | CC1CCC(=O)N1C | CCCCCCC=C | 1.52 | | | | | | | 1.94 | 1.80 | [62] |
| 106 | CC1CCC(=O)N1C | C1CCOC1 | 0.19 | | | | | | | 0.20 | 0.30 | [62] |
| 107 | CC1CCC(=O)N1C | CC(C)(C)OC | 0.58 | | | | | | | 1.00 | 0.99 | [62] |
| 108 | CC1CCC(=O)N1C | CCOC(C)(C)C | 0.78 | | | | | | | | 1.34 | [62] |
| 109 | CC1CCC(=O)N1C | CCC(C)(C)OC | 0.79 | | | | | | | | 1.11 | [62] |
| 110 | CC1CCC(=O)N1C | CCOCC | 0.49 | | | | | | | 0.96 | 0.98 | [62] |
| 111 | CC1CCC(=O)N1C | CC(C)OC(C)C | 0.80 | | | | | | | 1.49 | 1.47 | [62] |
| 112 | CC1CCC(=O)N1C | CC(C)=O | -0.07 | | | | | | | 0.07 | 0.05 | [62] |
| 113 | CC1CCC(=O)N1C | CCC(C)=O | -0.05 | | | | | | | 0.09 | 0.07 | [62] |
| 114 | CC1CCC(=O)N1C | CCCC(C)=O | 0.01 | | | | | | | 0.25 | 0.13 | [62] |
| 115 | CC1CCC(=O)N1C | CC=O | -0.12 | | | | | | | -0.12 | 0.04 | [62] |
| 116 | N#CCCCCCCC#N | CCCCCC | 2.78 | 1.79 | 1.80 | 2.77 | | | | | 2.34 | [47] |
| 117 | N#CCCCCCCC#N | C1CCCCC1 | 2.31 | 1.47 | 1.49 | 2.49 | | | | | 1.81 | [47] |
| 118 | N#CCCCCCCC#N | c1ccccc1 | 0.57 | 0.19 | 0.22 | 0.51 | | | | | 0.42 | [51 , 47] |
| 119 | N#CCCCCCCC#N | Cc1ccccc1 | 0.92 | 0.49 | 0.46 | 0.69 | | | | | 0.59 | [51] |
| 120 | N#CCCCCCCC#N | CCc1ccccc1 | 1.24 | 0.79 | 0.74 | 1.25 | | | | | 0.88 | [51] |
| 121 | N#CCCCCCCC#N | CC=C(C)C | 1.57 | 1.20 | 1.21 | 1.93 | | | | | 1.55 | [47] |
| 122 | N#CCCCCCCC#N | CC(=C)C=C | 1.02 | 0.57 | 0.65 | 0.81 | | | | | 0.82 | [47] |
| 123 | CCCCO | CO | 0.13 | 0.22 | 0.39 | 0.14 | 0.18 | -0.27 | 0.98 | 0.49 | 0.15 | [61] |
| 124 | CCCCO | CCO | 0.09 | 0.04 | 0.05 | 0.05 | 0.39 | -0.25 | 0.05 | -0.02 | -0.02 | [61 , 61] |
| 125 | CCCCO | C1COCCO1 | 0.22 | 0.92 | 0.86 | 1.08 | 0.28 | 0.42 | 0.09 | 0.81 | 0.88 | [61] |
| 126 | CCCCO | CCOCC | 0.04 | 0.59 | 0.58 | 0.77 | 0.56 | 0.66 | 2.00 | 0.60 | 0.70 | [61] |
| 127 | CCCCO | CC(C)=O | 0.31 | 0.72 | 0.75 | 0.85 | 0.87 | 0.19 | 0.17 | 0.91 | 0.86 | [61 , 61] |
| 128 | CCCCO | CCC(C)=O | 0.17 | 0.74 | 0.73 | 0.84 | 0.88 | 0.48 | 0.47 | 0.77 | 0.80 | [61 , 61] |
| 129 | CCCCO | CCCCl | 0.81 | 0.77 | 0.75 | 1.03 | 1.12 | | | | 1.04 | [61] |
| 130 | CCCCO | ClCCl | 0.09 | 0.57 | 0.62 | 0.69 | 0.31 | 0.14 | 0.06 | 0.66 | 0.65 | [61 , 61] |
| 131 | CCCCO | ClC(Cl)Cl | -0.01 | 0.43 | 0.38 | 0.42 | -0.02 | 0.36 | | 0.46 | 0.22 | [61 , 61] |
| 132 | CCCCO | ClC(Cl)(Cl)Cl | 1.26 | 1.00 | 0.95 | 1.04 | 1.35 | 1.45 | 0.93 | 1.10 | 0.97 | [61] |
| 133 | CCCCO | CCBr | 0.89 | 0.86 | 0.88 | 0.99 | 1.03 | 0.60 | | | 0.96 | [61] |
| 134 | CCCCO | CCC#N | 1.38 | 0.57 | 0.60 | 1.12 | 1.76 | 0.49 | -0.17 | 1.59 | 1.62 | [61] |
| 135 | CCCCO | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 5.91 | -1.51 | -1.71 | | | 4.47 | 4.25 | | 5.70 | [63] |
| 136 | CCCCO | CCI | 1.03 | 1.18 | 1.13 | 1.26 | 1.45 | | | | 1.21 | [61] |
| 137 | CCCCO | CCN(CC)CC | -0.09 | 0.38 | 0.29 | 0.11 | 0.14 | 2.08 | 0.99 | 0.51 | -0.17 | [61] |
| 138 | CCCCO | C(=S)=S | 1.30 | 1.12 | 1.11 | -1.39 | | 0.94 | -0.03 | | 1.12 | [61] |
| 139 | CCCCCl | CCCCC | 0.43 | 0.20 | 0.20 | 0.26 | 0.49 | 0.17 | 0.19 | 0.55 | 0.42 | [64] |
| 140 | CCCCCl | CCCCCC | 0.48 | 0.21 | 0.22 | 0.29 | 0.52 | 0.20 | 0.12 | 0.57 | 0.54 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 141 | CCCCCl | C1CCCCC1 | 0.40 | 0.23 | 0.19 | 0.36 | 0.44 | 0.04 | -0.17 | 0.53 | 0.48 | [61] |
| 142 | CCCCCl | c1ccccc1 | 0.06 | 0.03 | -0.07 | 0.04 | 0.19 | 0.01 | -0.19 | 0.04 | 0.02 | [64] |
| 143 | CCCCCl | Cc1ccccc1 | 0.09 | -0.04 | -0.16 | -0.01 | 0.12 | -0.01 | -0.16 | 0.09 | 0.05 | [64] |
| 144 | CCCCCl | CC(C)=O | 0.53 | 0.75 | 0.76 | 0.36 | 0.77 | -0.07 | -0.03 | 0.58 | 0.53 | [65 , 61] |
| 145 | CCCCCCCCCCCCCCCCCl | Clc1ccccc1 | 0.02 | -0.13 | 0.04 | -0.31 | | | | | -0.22 | [61] |
| 146 | CCCCCCl | CC(C)=O | 0.65 | 0.83 | 0.87 | 0.43 | | -0.17 | -0.07 | | 0.59 | [65] |
| 147 | CCCCCCCCC=C | CCCCC | -0.03 | -0.11 | -0.04 | 0.03 | | -0.26 | -0.19 | | -0.07 | [54] |
| 148 | CCCCCCCCC=C | CCCCCC | -0.01 | -0.05 | -0.01 | 0.04 | | -0.24 | -0.21 | | -0.15 | [54] |
| 149 | CCCCCCCCC=C | C1CCCCC1 | -0.04 | -0.08 | -0.03 | 0.08 | | -0.31 | -0.33 | | -0.05 | [54] |
| 150 | CCCCCCCCC=C | CCCC(C)C | -0.01 | -0.05 | -0.01 | 0.04 | | | | | 0.00 | [54] |
| 151 | CCCCCCCCC=C | CCCCCCC | 0.01 | 0.00 | 0.01 | 0.04 | | -0.21 | -0.24 | | 0.00 | [54] |
| 152 | CCCCCCCCC=C | CC(C)CC(C)C | 0.01 | 0.00 | 0.01 | 0.04 | | | | | 0.05 | [54] |
| 153 | CCCCCCCCC=C | CCCCCCCC | 0.02 | 0.03 | 0.03 | 0.05 | | -0.17 | -0.21 | | 0.03 | [54] |
| 154 | CCCCCCCCC=C | CC(C)C(C)C(C)C | 0.01 | 0.02 | 0.03 | 0.05 | | | | | 0.03 | [54] |
| 155 | CCCCCCCCC=C | CC(C)CCC(C)C | 0.02 | 0.02 | 0.03 | 0.05 | | | | | 0.06 | [54] |
| 156 | CCCCCCCCC=C | CCC1CCCCC1 | 0.01 | 0.02 | 0.02 | 0.09 | | | | | 0.00 | [54] |
| 157 | CCCCCCCCC=C | CCCCCCCCC | 0.03 | 0.04 | 0.04 | 0.05 | | -0.14 | -0.20 | | 0.09 | [54] |
| 158 | CCCCCC=C | CCOC(=O)C | 0.77 | 0.66 | 0.65 | 0.76 | | -0.07 | 0.29 | | 0.88 | [61] |
| 159 | CCCCCC=C | CCCCOC(=O)C | 0.50 | 0.36 | 0.39 | 0.49 | | -0.03 | 0.05 | | 0.68 | [61] |
| 160 | CCCCCC=C | CC#N | 2.91 | 2.46 | 2.54 | 2.83 | | 0.37 | 4.17 | | 2.99 | [61] |
| 161 | CCCCCC=C | CCC#N | 2.13 | 1.53 | 1.55 | 1.89 | | 0.34 | 1.88 | | 2.45 | [61] |
| 162 | CCCCCC=C | C[N+]([O-])=O | 2.60 | 2.86 | 2.91 | 2.75 | | 0.48 | 4.91 | | 3.12 | [61] |
| 163 | CCCCCCCCCCCCCCCC=C | CCCCl | 0.13 | -0.40 | -0.15 | 0.03 | | | | | 0.10 | [61] |
| 164 | CCCCCCCCCCCCCCCC=C | CCCCCl | 0.12 | -0.31 | -0.12 | 0.03 | | | | | 0.10 | [61] |
| 165 | CCCCC=C | CCCCC | 0.04 | 0.06 | 0.06 | 0.08 | | -0.21 | -0.21 | 0.02 | 0.03 | [54] |
| 166 | CCCCC=C | CCCCCC | 0.05 | 0.07 | 0.07 | 0.06 | | -0.17 | -0.19 | 0.02 | 0.10 | [54] |
| 167 | CCCCC=C | C1CCCCC1 | 0.05 | 0.10 | 0.06 | 0.19 | | -0.11 | -0.02 | 0.07 | 0.19 | [54 , 61] |
| 168 | CCCCC=C | CCCC(C)C | 0.05 | 0.07 | 0.07 | 0.06 | | | | 0.05 | 0.07 | [54 , 61] |
| 169 | CCCCC=C | CCCCCCC | 0.05 | 0.06 | 0.07 | 0.05 | | -0.14 | -0.14 | 0.01 | 0.13 | [54 , 61] |
| 170 | CCCCC=C | CC(C)CC(C)C | 0.04 | 0.06 | 0.07 | 0.05 | | | | 0.07 | 0.20 | [54] |
| 171 | CCCCC=C | CCCCCCCC | 0.04 | 0.04 | 0.07 | 0.03 | | -0.11 | -0.11 | 0.00 | 0.17 | [54 , 61] |
| 172 | CCCCC=C | CC(C)C(C)C(C)C | 0.02 | 0.04 | 0.07 | 0.03 | | | | | 0.16 | [54 , 61] |
| 173 | CCCCC=C | CC(C)CCC(C)C | 0.03 | 0.04 | 0.07 | 0.03 | | | | | 0.14 | [54] |
| 174 | CCCCC=C | CCC1CCCCC1 | 0.05 | 0.10 | 0.07 | 0.17 | | | | 0.09 | 0.25 | [54 , 61] |
| 175 | CCCCC=C | CCCCCCCCC | 0.02 | 0.00 | 0.06 | 0.01 | | -0.06 | -0.07 | -0.01 | 0.14 | [54 , 61] |
| 176 | CCCCCCCCCCCCCCCCI | Clc1ccccc1 | | -0.31 | -0.13 | -0.39 | | | | | -0.22 | [61] |
| 177 | Cc1cccc2ccccc12 | CCCCC | 0.71 | 0.60 | 0.29 | 1.02 | | 0.94 | 2.28 | | 1.12 | [47] |
| 178 | Cc1cccc2ccccc12 | CCCCCC | 0.80 | 0.72 | 0.37 | 1.05 | | 0.99 | 2.02 | | 1.10 | [47] |
| 179 | Cc1cccc2ccccc12 | C1CCCCC1 | 0.57 | 0.41 | 0.30 | 0.84 | | 0.25 | 0.81 | | 0.79 | [47 , 61] |
| 180 | Cc1cccc2ccccc12 | c1ccccc1 | -0.04 | -0.13 | -0.08 | -0.01 | | -0.20 | 0.06 | | 0.22 | [47] |
| 181 | Cc1cccc2ccccc12 | CC=C(C)C | 0.34 | 0.55 | 0.16 | 0.73 | | 0.76 | 1.92 | | 0.80 | [47] |
| 182 | Cc1cccc2ccccc12 | CC(=C)C=C | 0.16 | 0.21 | 0.02 | 0.28 | | | | | 0.52 | [47 , 61] |
| 183 | CCC[N+]([O-])=O | CCCCC | 1.78 | 1.31 | 1.31 | 1.57 | | 1.25 | 1.56 | 1.88 | 1.66 | [54 , 66 , 47] |
| 184 | CCC[N+]([O-])=O | CCC(C)C | 1.71 | 1.31 | 1.31 | 1.57 | | 1.39 | 1.98 | | 1.65 | [47] |
| 185 | CCC[N+]([O-])=O | CCCCCC | 2.03 | 1.49 | 1.51 | 1.72 | | 1.41 | 1.39 | 2.07 | 1.85 | [54 , 66 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 186 | CCC[N+]([O-])=O | C1CCCCC1 | 1.74 | 1.34 | 1.28 | 1.80 | | 1.03 | 0.60 | 1.85 | 1.49 | [54 , 66 , 47] |
| 187 | CCC[N+]([O-])=O | CCCC(C)C | 1.96 | 1.49 | 1.51 | 1.72 | | | | 2.11 | 1.90 | [54] |
| 188 | CCC[N+]([O-])=O | CCCCCCC | 2.26 | 1.65 | 1.70 | 1.86 | | 1.57 | 1.23 | 2.27 | 2.15 | [54] |
| 189 | CCC[N+]([O-])=O | CC(C)CC(C)C | 2.11 | 1.65 | 1.70 | 1.86 | | | | 2.34 | 2.05 | [54] |
| 190 | CCC[N+]([O-])=O | CCCCCCCC | 2.49 | 1.80 | 1.89 | 2.00 | | 1.75 | 1.16 | 2.46 | 2.36 | [54] |
| 191 | CCC[N+]([O-])=O | CC(C)C(C)C(C)C | 2.21 | 1.79 | 1.88 | 2.00 | | | | | 2.11 | [54] |
| 192 | CCC[N+]([O-])=O | CC(C)CCC(C)C | 2.37 | 1.79 | 1.88 | 2.00 | | | | | 2.19 | [54] |
| 193 | CCC[N+]([O-])=O | CCC1CCCCC1 | 2.16 | 1.68 | 1.66 | 1.98 | | | | 2.31 | 2.10 | [54] |
| 194 | CCC[N+]([O-])=O | CCCCCCCCC | 2.72 | 1.93 | 2.06 | 2.14 | | 1.93 | 1.09 | 2.65 | 2.54 | [54] |
| 195 | CCC[N+]([O-])=O | c1ccccc1 | 0.51 | 0.46 | 0.31 | 0.32 | | 0.76 | 0.10 | 0.39 | 0.03 | [47] |
| 196 | CCC[N+]([O-])=O | CC=C(C)C | 1.16 | 1.17 | 1.16 | 1.15 | | 0.68 | 1.33 | | 1.06 | [47] |
| 197 | CCC[N+]([O-])=O | CC(=C)C=C | 0.77 | 0.90 | 0.90 | 0.48 | | | | | 0.60 | [47] |
| 198 | CCCCCCCCO | CCO | 0.29 | 0.15 | 0.21 | 0.17 | 0.44 | -0.33 | 1.68 | 0.09 | 0.13 | [61] |
| 199 | CCCCCCCCO | CCOC(=O)C | 0.23 | 0.55 | 0.64 | 0.70 | 0.92 | -0.31 | -0.21 | 0.97 | 0.85 | [61] |
| 200 | CCCCCCCCO | C1COCCO1 | 0.15 | 0.82 | 0.74 | 0.73 | 0.22 | -0.05 | -0.40 | 0.70 | 0.69 | [61] |
| 201 | CCCCCCCCO | CC(C)=O | 0.38 | 0.55 | 0.71 | 0.78 | 0.91 | -0.22 | -0.45 | 0.94 | 0.93 | [61] |
| 202 | CCCCCCCCO | CCC(C)=O | 0.15 | 0.54 | 0.65 | 0.74 | 0.85 | -0.04 | -0.24 | 0.69 | 0.74 | [61] |
| 203 | CCCCCCCCO | ClCCl | -0.07 | 0.11 | 0.32 | 0.54 | 0.10 | -0.31 | -0.53 | 0.19 | 0.45 | [61 , 67 , 68] |
| 204 | CCCCCCCCO | CC(Cl)Cl | -0.07 | 0.20 | 0.33 | 0.48 | | 0.28 | 0.28 | 0.62 | 0.70 | [67] |
| 205 | CCCCCCCCO | ClCCCl | 0.35 | 0.69 | 0.82 | 1.10 | 0.43 | 0.06 | -0.43 | 0.74 | 0.99 | [67] |
| 206 | CCCCCCCCO | CC(Cl)CCl | 0.54 | 0.60 | 0.67 | 0.89 | 0.97 | | | | 0.95 | [67] |
| 207 | CCCCCCCCO | ClC(Cl)Cl | 0.55 | 0.10 | 0.22 | 0.22 | -0.34 | -0.16 | | -0.19 | 0.00 | [61 , 67 , 68] |
| 208 | CCCCCCCCO | CC(Cl)(Cl)Cl | -0.34 | 0.20 | 0.28 | 0.31 | 0.67 | | | | 0.68 | [67] |
| 209 | CCCCCCCCO | ClCC(Cl)Cl | 0.39 | 0.76 | 0.82 | 1.01 | | -0.11 | | | 0.62 | [67 , 68] |
| 210 | CCCCCCCCO | ClC(Cl)(Cl)Cl | 0.04 | 0.40 | 0.49 | 0.53 | 0.87 | 0.63 | 0.13 | 0.46 | 0.58 | [61 , 67 , 68] |
| 211 | CCCCCCCCO | CCBr | 0.63 | 0.41 | 0.59 | 0.62 | 0.71 | 0.01 | | | 0.68 | [61] |
| 212 | CCCCCCCCO | BrCBr | 0.68 | 1.48 | 1.65 | 1.10 | | -0.33 | -0.48 | | 0.77 | [67 , 68] |
| 213 | CCCCCCCCO | ClC(Br)Br | 0.74 | 2.32 | 2.41 | 1.62 | | | | | 0.75 | [68] |
| 214 | CCCCCCCCO | CCC#N | 1.54 | 0.51 | 0.68 | 1.13 | 1.81 | 0.06 | -0.42 | 1.61 | 1.82 | [61] |
| 215 | CCCCCCCCO | CCI | 0.79 | 0.66 | 0.78 | 0.79 | 1.03 | | | | 0.82 | [61] |
| 216 | CCCCCCCCO | C(=S)=S | 0.77 | 0.41 | 0.62 | -1.47 | | 0.29 | -0.56 | | 0.55 | [61] |
| 217 | CCCCCCC=C | CCCCC | 0.01 | -0.02 | 0.00 | 0.20 | | -0.21 | -0.21 | 0.00 | -0.03 | [54 , 61] |
| 218 | CCCCCCC=C | CCCCCC | 0.03 | 0.02 | 0.03 | 0.18 | | -0.17 | -0.21 | -0.01 | 0.02 | [54] |
| 219 | CCCCCCC=C | C1CCCCC1 | 0.00 | 0.01 | 0.01 | 0.14 | | -0.20 | -0.19 | 0.01 | 0.04 | [54 , 61] |
| 220 | CCCCCCC=C | CCCC(C)C | 0.02 | 0.02 | 0.03 | 0.18 | | | | 0.04 | 0.04 | [54] |
| 221 | CCCCCCC=C | CCCCCCC | 0.03 | 0.04 | 0.04 | 0.17 | | -0.14 | -0.20 | 0.01 | 0.05 | [54 , 61] |
| 222 | CCCCCCC=C | CC(C)CC(C)C | 0.03 | 0.04 | 0.04 | 0.17 | | | | 0.08 | 0.07 | [54] |
| 223 | CCCCCCC=C | CCCCCCCC | 0.04 | 0.04 | 0.04 | 0.15 | | -0.11 | -0.17 | 0.02 | 0.12 | [54] |
| 224 | CCCCCCC=C | CC(C)C(C)C(C)C | 0.02 | 0.04 | 0.04 | 0.15 | | | | | 0.07 | [54 , 61] |
| 225 | CCCCCCC=C | CC(C)CCC(C)C | 0.03 | 0.04 | 0.04 | 0.15 | | | | | 0.09 | [54] |
| 226 | CCCCCCC=C | CCC1CCCCC1 | 0.03 | 0.07 | 0.04 | 0.12 | | | | 0.05 | 0.11 | [54 , 61] |
| 227 | CCCCCCC=C | CCCCCCCCC | 0.04 | 0.03 | 0.04 | 0.12 | | -0.07 | -0.15 | 0.03 | 0.17 | [54] |
| 228 | CCCCCO | CCO | 0.14 | 0.07 | 0.09 | 0.09 | 0.20 | -0.26 | 0.52 | 0.02 | 0.08 | [61] |
| 229 | CCCCCO | CC(C)=O | 0.35 | 0.67 | 0.74 | 0.83 | 0.88 | 0.00 | -0.14 | 0.93 | 0.94 | [61] |
| 230 | CCCCCO | CCC(C)=O | 0.17 | 0.68 | 0.70 | 0.82 | 0.87 | 0.23 | 0.11 | 0.71 | 0.90 | [61] |

Continued on next page

**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 231 | CCCCCO | ClCCl | 0.06 | 0.43 | 0.52 | 0.65 | 0.29 | -0.04 | -0.24 | 0.59 | 0.80 | [61] |
| 232 | CCCCCO | ClC(Cl)Cl | -0.11 | 0.33 | 0.33 | 0.36 | -0.13 | 0.16 | | 0.40 | 0.41 | [61] |
| 233 | CCCO | CCO | 0.02 | 0.01 | 0.02 | 0.02 | 0.34 | -0.24 | -0.12 | -0.02 | -0.08 | [61] |
| 234 | CCCO | C1COCCO1 | 0.13 | 0.94 | 0.91 | 1.24 | 0.48 | 0.67 | 0.28 | 0.91 | 0.88 | [61] |
| 235 | CCCO | CCC(C)=O | 0.11 | 0.82 | 0.77 | 0.88 | 1.13 | 0.69 | 0.68 | 0.90 | 0.82 | [61] |
| 236 | CCCO | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 5.64 | -1.27 | -1.47 | -4.61 | | | | | 5.42 | [63] |
| 237 | CCCO | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 6.22 | -1.43 | -1.71 | | | 5.40 | 4.16 | | 5.99 | [63] |
| 238 | CCCO | CCN(CC)CC | 0.02 | 0.60 | 0.49 | 0.29 | 0.22 | 2.64 | 1.18 | 0.42 | -0.11 | [61] |
| 239 | CCN(CC)CCN | C1CCCCC1 | | 0.47 | 0.46 | 0.45 | | | | | 0.63 | [69] |
| 240 | CCN(CC)CCN | CCCCCCC | | 0.66 | 0.66 | 0.72 | | | | | 0.69 | [70] |
| 241 | CC(C)CC(C)(C)C | CCCCC | -0.03 | -0.07 | -0.04 | -0.01 | -0.07 | -0.30 | -0.29 | -0.08 | -0.09 | [54 , 61] |
| 242 | CC(C)CC(C)(C)C | CCCCCC | -0.01 | -0.03 | -0.01 | -0.01 | 0.01 | -0.24 | -0.21 | -0.01 | -0.01 | [54 , 61] |
| 243 | CC(C)CC(C)(C)C | C1CCCCC1 | -0.01 | -0.02 | -0.03 | 0.03 | -0.03 | -0.13 | 0.17 | 0.20 | 0.06 | [54] |
| 244 | CC(C)CC(C)(C)C | CCCC(C)C | -0.01 | -0.03 | -0.01 | -0.01 | 0.05 | | | -0.04 | -0.02 | [54 , 61] |
| 245 | CC(C)CC(C)(C)C | CCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.09 | -0.17 | -0.13 | 0.05 | 0.07 | [54] |
| 246 | CC(C)CC(C)(C)C | CC(C)CC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | 0.12 | | | -0.02 | 0.02 | [54 , 61] |
| 247 | CC(C)CC(C)(C)C | CCCCCCCC | 0.00 | 0.00 | 0.00 | 0.00 | 0.21 | -0.12 | -0.06 | 0.11 | 0.05 | [54 , 61 , 61] |
| 248 | CC(C)CC(C)(C)C | CC(C)C(C)C(C)C | 0.00 | 0.00 | 0.00 | 0.00 | -0.08 | | | | 0.05 | [54 , 61] |
| 249 | CC(C)CC(C)(C)C | CC(C)CCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | | | | | 0.06 | [54] |
| 250 | CC(C)CC(C)(C)C | CCC1CCCCC1 | 0.02 | 0.05 | 0.00 | 0.05 | | | | 0.27 | 0.15 | [54 , 61] |
| 251 | CC(C)CC(C)(C)C | CCCCCCCCC | 0.00 | 0.00 | 0.00 | 0.00 | 0.41 | -0.06 | 0.00 | 0.17 | 0.18 | [54 , 61] |
| 252 | CC(C)CC(C)(C)C | CCC(C)CCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | | | | | 0.01 | [61] |
| 253 | CC(C)CC(C)(C)C | Cc1ccccc1 | 0.51 | 0.43 | 0.34 | 0.40 | 0.52 | 0.10 | 0.77 | 0.57 | 0.45 | [61] |
| 254 | CC(C)CC(C)(C)C | CCCC=C | 0.01 | -0.02 | 0.04 | 0.00 | 0.02 | -0.21 | -0.31 | -0.08 | -0.01 | [61] |
| 255 | CC(C)CC(C)(C)C | CC(C)C=C | 0.01 | -0.02 | 0.04 | 0.00 | | | | | -0.03 | [61] |
| 256 | CC(C)CC(C)(C)C | CC(=C)C=C | 0.24 | 0.06 | 0.14 | 0.22 | 0.16 | | | | -0.02 | [61] |
| 257 | CC(C)CC(C)(C)C | CO | 4.32 | 2.86 | 3.10 | 4.23 | 4.15 | 0.78 | 15.19 | 5.25 | 4.28 | [61] |
| 258 | CC(C)CC(C)(C)C | CCO | 4.13 | 3.19 | 3.17 | 3.80 | 3.73 | 1.04 | 9.67 | 4.31 | 3.80 | [61] |
| 259 | CC(C)CC(C)(C)C | CCOC(=O)C | 1.19 | 1.05 | 1.10 | 1.21 | 1.33 | 0.12 | 0.97 | 1.51 | 1.12 | [61] |
| 260 | CC(C)CC(C)(C)C | C1CCOC1 | 0.43 | 0.41 | 0.44 | 0.28 | 0.17 | 0.17 | 1.47 | 0.47 | 0.30 | [61] |
| 261 | CC(C)CC(C)(C)C | C1COCCO1 | 1.08 | 1.85 | 1.67 | 1.07 | 1.09 | 0.38 | 2.28 | 1.54 | 1.27 | [61] |
| 262 | CC(C)CC(C)(C)C | CC(C)=O | 1.93 | 1.71 | 1.82 | 1.71 | 1.87 | 0.25 | 1.78 | 1.71 | 1.93 | [61] |
| 263 | CC(C)CC(C)(C)C | CCC(C)=O | 1.57 | 1.58 | 1.65 | 1.59 | 1.47 | 0.26 | 1.24 | 1.36 | 1.43 | [61] |
| 264 | CC(C)CC(C)(C)C | CCCCl | 0.44 | 0.05 | 0.14 | 0.25 | 0.36 | | | | 0.38 | [61] |
| 265 | CC(C)CC(C)(C)C | ClCCl | 0.61 | 0.24 | 0.41 | 0.63 | 0.63 | 0.01 | 1.93 | 0.72 | 0.74 | [61] |
| 266 | CC(C)CC(C)(C)C | ClC(Cl)Cl | 0.31 | 0.28 | 0.39 | 0.36 | 0.42 | 0.03 | | 0.45 | 0.41 | [61] |
| 267 | CC(C)CC(C)(C)C | CCBr | 0.81 | 0.46 | 0.59 | 0.38 | 0.31 | -0.04 | | | 0.48 | [61] |
| 268 | CC(C)CC(C)(C)C | CCC#N | 2.79 | 2.09 | 2.22 | 2.25 | 2.61 | 0.50 | 3.29 | 2.60 | 2.94 | [61] |
| 269 | CC(C)CC(C)(C)C | CC[N+](=O)[O-] | 2.72 | 2.53 | 2.64 | 1.96 | | 0.68 | 4.46 | | 2.89 | [61] |
| 270 | CC(C)CC(C)(C)C | CCI | 0.87 | 0.54 | 0.65 | 0.60 | 0.67 | | | | 0.62 | [61] |
| 271 | CC(C)CC(C)(C)C | C(=S)=S | 0.43 | 0.16 | 0.34 | 0.23 | | 0.02 | 2.15 | | 0.28 | [61] |
| 272 | CC(=O)C(C)=O | CCCCCCC | 2.16 | 3.81 | 3.85 | 4.27 | | 0.55 | 0.14 | | 2.60 | [71] |
| 273 | CC(C)C(C)C | C1CCCC1 | -0.01 | -0.01 | -0.02 | 0.08 | | | | 0.12 | 0.03 | [72] |
| 274 | CC1CC(C)[S](=O)(=O)C1 | CCCCCC | 2.60 | 1.79 | 1.74 | 2.25 | | | | | 2.56 | [47 , 73] |
| 275 | CC1CC(C)[S](=O)(=O)C1 | c1ccccc1 | 0.54 | 0.21 | 0.25 | 0.28 | | | | | 0.18 | [47 , 73] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 276 | CC(=O)CC(C)=O | CCCCC | 2.57 | 2.37 | 2.37 | 2.89 | | 1.05 | 1.35 | | 1.56 | [74] |
| 277 | CC(=O)CC(C)=O | CCCC=C | 1.72 | 1.80 | 1.80 | 2.09 | | 0.62 | 1.35 | | 1.01 | [74] |
| 278 | CC(=O)CCC(C)=O | CCCCCCC | 2.78 | 2.60 | 2.60 | 3.01 | | | | | 2.85 | [71] |
| 279 | Cc1cccc(C)n1 | CCCCCCC | 1.00 | 0.76 | 0.51 | 0.56 | | | | 1.26 | 0.91 | [75] |
| 280 | Cc1cccc(C)n1 | CCCCCCCC | 1.10 | 0.80 | 0.56 | 0.54 | | | | 1.35 | 1.10 | [75] |
| 281 | CCC(C)O | CCCCCC | 1.48 | 1.35 | 1.28 | 1.39 | 1.80 | 1.83 | 1.80 | 1.59 | 2.02 | [76] |
| 282 | CCC(C)O | c1ccccc1 | 0.90 | 1.05 | 0.76 | 1.16 | 1.29 | 0.96 | 0.28 | 1.04 | 1.28 | [77] |
| 283 | CCC(C)=O | CCCCCC | 1.57 | 1.38 | 1.40 | 1.47 | 1.34 | 0.77 | 0.49 | 1.43 | 1.38 | [47 , 54 , 61 , 61 , 73] |
| 284 | CCC(C)=O | c1ccccc1 | 0.25 | 0.25 | 0.09 | 0.18 | 0.21 | 0.42 | -0.19 | 0.13 | 0.11 | [47 , 47 , 80] |
| 285 | CCC(C)=O | CCCCC | 1.37 | 1.22 | 1.22 | 1.35 | 1.18 | 0.67 | 0.59 | 1.30 | 1.26 | [54 , 61 , 61] |
| 286 | CCC(C)=O | C1CCCCC1 | 1.35 | 1.26 | 1.19 | 1.50 | 1.12 | 0.55 | 0.02 | 1.40 | 1.38 | [54 , 61 , 78 , 79] |
| 287 | CCC(C)=O | CCCC(C)C | 1.51 | 1.38 | 1.40 | 1.47 | 1.35 | | | 1.45 | 1.36 | [54 , 61 , 61] |
| 288 | CCC(C)=O | CCCCCCC | 1.76 | 1.52 | 1.57 | 1.59 | 1.48 | 0.87 | 0.40 | 1.57 | 1.45 | [54 , 61 , 78] |
| 289 | CCC(C)=O | CC(C)CC(C)C | 1.62 | 1.52 | 1.57 | 1.59 | 1.47 | | | 1.59 | 3.00 | [54 , 61 , 61] |
| 290 | CCC(C)=O | CC1CCCCC1 | 1.50 | 1.42 | 1.36 | 1.54 | 1.17 | 0.64 | 0.20 | 1.49 | 1.45 | [61] |
| 291 | CCC(C)=O | CCCCCCCC | 1.94 | 1.64 | 1.74 | 1.71 | 1.66 | 0.98 | 0.36 | 1.70 | 1.67 | [54 , 61 , 61 , 61] |
| 292 | CCC(C)=O | CC(C)C(C)C(C)C | 1.71 | 1.64 | 1.74 | 1.71 | 1.36 | | | | 1.52 | [54 , 61 , 61] |
| 293 | CCC(C)=O | CC(C)CCC(C)C | 1.83 | 1.64 | 1.74 | 1.71 | | | | | 1.59 | [54] |
| 294 | CCC(C)=O | CCC1CCCCC1 | 1.68 | 1.56 | 1.53 | 1.67 | | | | 1.68 | 1.57 | [54 , 61 , 61] |
| 295 | CCC(C)=O | CCCCCCCCC | 2.12 | 1.76 | 1.90 | 1.83 | 1.93 | 1.09 | 0.32 | 1.83 | 1.82 | [54 , 61 , 61] |
| 296 | CCC(C)=O | Cc1ccccc1 | 0.43 | 0.30 | 0.12 | 0.35 | 0.27 | 0.39 | -0.13 | 0.29 | 0.29 | [61] |
| 297 | CCC(C)=O | CCO | 0.41 | 0.89 | 0.80 | 0.86 | 0.97 | 0.40 | 1.72 | 0.99 | 0.86 | [61] |
| 298 | CCC(C)=O | CCOC(=O)C | 0.04 | 0.06 | 0.06 | 0.10 | 0.29 | -0.17 | -0.22 | 0.00 | 0.11 | [61] |
| 299 | CCC(C)=O | C1COCCO1 | 0.04 | 0.45 | 0.27 | 0.24 | -0.26 | 0.28 | -0.13 | 0.13 | 0.16 | [61] |
| 300 | CCC(C)=O | C[N+]([O-])=O | -0.06 | 0.01 | 0.05 | 0.00 | 0.71 | -0.04 | 0.98 | -0.03 | 0.25 | [61] |
| 301 | CCC(C)=O | CCN(CC)CC | 0.94 | 0.94 | 0.99 | 1.07 | 1.05 | 0.77 | -0.05 | 1.06 | 1.00 | [61] |
| 302 | CCCCOCCO | CCCCCC | 1.10 | 1.14 | 1.14 | 1.46 | 1.48 | 1.25 | 1.66 | | 1.48 | [81] |
| 303 | CCCCOCCO | C1CCCCC1 | 0.93 | 0.99 | 0.96 | 1.33 | 1.26 | 0.90 | 0.60 | | 1.08 | [81] |
| 304 | CCCCOCCO | CC1CCCC1 | 0.93 | 0.99 | 0.95 | 1.15 | 1.16 | | | | 1.08 | [81] |
| 305 | CCCCOCCO | CCCCCCC | 1.25 | 1.31 | 1.31 | 1.61 | 1.62 | 1.42 | 1.44 | | 1.52 | [81] |
| 306 | CCCCOCCO | CC1CCCCC1 | 1.06 | 1.18 | 1.12 | 1.40 | 1.30 | 0.99 | 1.01 | | 1.26 | [81] |
| 307 | CCCCOCCO | CCCCCCCC | 1.39 | 1.47 | 1.47 | 1.75 | 1.81 | 1.61 | 1.35 | | 1.68 | [81] |
| 308 | CCCCOCCO | C1CCCCCCC1 | 1.16 | 1.35 | 1.29 | 1.80 | 1.32 | 1.35 | 0.33 | | 1.44 | [81] |
| 309 | CCCCOCCO | CCCCCCCCC | 1.53 | 1.61 | 1.62 | 1.89 | 2.08 | 1.79 | 1.26 | | 1.81 | [81] |
| 310 | CCCCOCCO | CCCCCCCCCC | 1.66 | 1.74 | 1.76 | 2.03 | 2.32 | 1.98 | 1.27 | | 2.05 | [81] |
| 311 | CCCCOCCO | CCCCCCCCCCC | 1.79 | 1.86 | 1.90 | 2.17 | 2.12 | | | | 2.34 | [81] |
| 312 | CCCCOCCO | c1ccccc1 | 0.34 | 0.30 | 0.22 | 0.69 | 0.55 | 0.52 | -0.03 | | 0.41 | [81] |
| 313 | CCCCOCCO | Cc1ccccc1 | 0.51 | 0.58 | 0.45 | 0.79 | 0.62 | 0.62 | 0.12 | | 0.59 | [81] |
| 314 | CCCCOCCO | Cc1cccc(C)c1 | 0.61 | 0.78 | 0.63 | 0.89 | 0.75 | 0.65 | 0.18 | | 0.79 | [81] |
| 315 | CCCCOCCO | Cc1ccc(C)cc1 | 0.62 | 0.78 | 0.63 | 0.89 | 0.69 | 0.62 | 0.24 | | 1.21 | [81] |
| 316 | CCCCOCCO | CCc1ccccc1 | 0.62 | 0.72 | 0.57 | 1.04 | 0.79 | 0.92 | 0.25 | | 0.77 | [81] |
| 317 | CCCCOCCO | C1CCC=CC1 | 0.63 | 0.91 | 0.87 | 0.92 | 0.92 | 0.20 | 0.17 | | 0.84 | [81] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 318 | CCCCOCCO | C=CCCCCC=C | 0.76 | 1.38 | 1.37 | 1.31 | | | | | 0.83 | [81] |
| 319 | CCCCOCCO | CC(C)(C)Cl | 0.34 | 0.37 | 0.39 | 0.92 | 0.89 | | | | 0.57 | [81] |
| 320 | CCCCOCCO | Clc1ccccc1 | 0.33 | 0.62 | 0.46 | 0.49 | 0.65 | 0.62 | -0.19 | | 0.38 | [81] |
| 321 | CCCCOCCO | Clc1ccccc1Cl | 0.35 | 1.00 | 0.79 | 0.35 | 0.79 | | | | 0.64 | [81] |
| 322 | CCCCOCCO | Brc1ccccc1 | 0.87 | 0.43 | 0.27 | 1.02 | 0.75 | 0.69 | -0.22 | | 0.64 | [81] |
| 323 | CCCCOCCO | Fc1ccccc1 | 0.30 | 0.18 | 0.10 | 0.52 | | 0.48 | -0.24 | | 0.25 | [81] |
| 324 | OCCCl | CCCCCC | 3.15 | 2.45 | 2.37 | 3.32 | | 3.00 | 3.07 | | 3.76 | [47 , 73] |
| 325 | OCCCl | c1ccccc1 | 1.44 | 1.08 | 0.70 | 1.26 | | 1.57 | 1.26 | | 1.82 | [47 , 73] |
| 326 | CCOCCO | C1CCCCC1 | 1.62 | 1.47 | 1.37 | 1.89 | 1.84 | 1.70 | 1.58 | 2.30 | 1.72 | [47 , 73] |
| 327 | CCCCCC(C)=O | CCCCC | 0.68 | 0.61 | 0.63 | 0.82 | | 0.18 | 0.31 | | 0.63 | [54] |
| 328 | CCCCCC(C)=O | CCCCCC | 0.80 | 0.75 | 0.75 | 0.90 | | 0.23 | 0.22 | | 0.79 | [54] |
| 329 | CCCCCC(C)=O | C1CCCCC1 | 0.66 | 0.64 | 0.62 | 0.91 | | 0.06 | -0.22 | | 0.69 | [54] |
| 330 | CCCCCC(C)=O | CCCC(C)C | 0.77 | 0.75 | 0.75 | 0.90 | | | | | 0.78 | [54] |
| 331 | CCCCCC(C)=O | CCCCCCC | 0.91 | 0.86 | 0.86 | 0.97 | | 0.29 | 0.13 | | 0.88 | [54] |
| 332 | CCCCCC(C)=O | CC(C)CC(C)C | 0.83 | 0.86 | 0.86 | 0.97 | | | | | 0.87 | [54] |
| 333 | CCCCCC(C)=O | CCCCCCCC | 1.01 | 0.97 | 0.97 | 1.05 | | 0.34 | 0.10 | | 1.00 | [54] |
| 334 | CCCCCC(C)=O | CC(C)C(C)C(C)C | 0.88 | 0.96 | 0.97 | 1.05 | | | | | 0.89 | [54] |
| 335 | CCCCCC(C)=O | CC(C)CCC(C)C | 0.95 | 0.97 | 0.97 | 1.05 | | | | | 0.95 | [54] |
| 336 | CCCCCC(C)=O | CCC1CCCCC1 | 0.85 | 0.89 | 0.85 | 1.02 | | | | | 0.88 | [54] |
| 337 | CCCCCC(C)=O | CCCCCCCCC | 1.11 | 1.05 | 1.06 | 1.12 | | 0.41 | 0.08 | | 1.13 | [54] |
| 338 | CCCC#CC | CCCCCCCC | 0.34 | 0.17 | 0.20 | 0.34 | | | | | 0.29 | [82] |
| 339 | CC(C)OCCO | CCCCCC | 1.59 | 1.36 | 1.36 | 1.70 | 1.67 | 1.76 | 2.35 | | 1.63 | [83] |
| 340 | CC(C)OCCO | C1CCCCC1 | 1.36 | 1.21 | 1.14 | 1.57 | 1.41 | 1.34 | 1.17 | | 1.37 | [83] |
| 341 | CC(C)OCCO | CCCCCCC | 1.79 | 1.54 | 1.54 | 1.86 | 1.85 | 2.00 | 2.10 | | 1.79 | [83] |
| 342 | CC(C)OCCO | CCCCCCCC | 1.99 | 1.71 | 1.72 | 2.03 | 2.08 | 2.24 | 1.99 | | 1.91 | [83] |
| 343 | CC(C)OCCO | CCCCCCCCC | 2.19 | 1.86 | 1.89 | 2.19 | 2.39 | 2.48 | 1.89 | | 2.17 | [83] |
| 344 | CC(C)OCCO | c1ccccc1 | 0.57 | 0.42 | 0.30 | 0.85 | 0.59 | 0.88 | 0.39 | | 0.47 | [83] |
| 345 | CC(C)OCCO | Cc1cccc(C)c1 | 0.97 | 0.95 | 0.76 | 1.08 | 0.89 | 1.05 | 0.63 | | 0.90 | [83] |
| 346 | CC(C)OCCO | Cc1ccc(C)cc1 | 0.98 | 0.95 | 0.76 | 1.08 | 0.82 | 1.02 | 0.70 | | 0.96 | [83] |
| 347 | CC(C)OCCO | Cc1ccccc1C | 0.92 | 0.95 | 0.76 | 1.08 | 0.82 | 1.02 | 0.62 | | 0.98 | [83] |
| 348 | CC(C)OCCO | CCc1ccccc1 | 0.97 | 0.87 | 0.70 | 1.24 | 0.91 | 1.36 | 0.71 | | 0.99 | [83] |
| 349 | CC(C)OCCO | CCCCCC#C | 0.39 | 0.14 | 0.15 | 1.08 | | | | | 0.80 | [83] |
| 350 | CC(C)OCCO | CCCCCCC#C | 0.55 | 0.22 | 0.24 | 1.22 | | | | | 1.10 | [83] |
| 351 | CC(C)OCCO | CC(C)O | 0.03 | 0.46 | 0.41 | -0.05 | 1.00 | -0.25 | -0.24 | | 0.17 | [83] |
| 352 | CC(C)OCCO | CCCCOC(=O)C | 0.51 | 0.64 | 0.64 | 0.41 | 0.75 | 0.37 | 0.93 | | 0.99 | [83] |
| 353 | CC(C)OCCO | C1CCOC1 | -0.09 | 0.16 | 0.16 | 0.77 | -0.11 | -0.13 | 0.07 | | 0.01 | [83] |
| 354 | CC(C)OCCO | C1COCCO1 | 0.19 | 0.11 | -0.07 | 0.53 | 0.06 | 0.29 | -0.14 | | 0.23 | [83] |
| 355 | CC(C)OCCO | CCC(C)=O | 0.19 | 0.73 | 0.75 | 0.52 | 0.56 | 0.09 | 0.21 | | 0.39 | [83] |
| 356 | CC(C)OCCO | ClCCl | -0.60 | -0.21 | -0.12 | -0.20 | -0.27 | -0.11 | -0.20 | | -0.46 | [83] |
| 357 | CC(C)OCCO | CC(Cl)CCl | 0.24 | -0.33 | -0.33 | 0.89 | 0.61 | | | | 0.42 | [83] |
| 358 | CC(C)OCCO | Clc1ccccc1 | 0.57 | 0.74 | 0.55 | 0.62 | 0.64 | 0.85 | 0.10 | | 0.48 | [83] |
| 359 | CC(C)OCCO | Brc1ccccc1 | 1.11 | 0.49 | 0.29 | 1.15 | 0.74 | 0.86 | -0.20 | | 0.57 | [83] |
| 360 | CC(C)OCCO | CC#N | 0.87 | 0.84 | 0.97 | 0.76 | 0.80 | -0.01 | -0.26 | | 0.71 | [83] |
| 361 | CC(C)OCCO | Fc1ccccc1 | 0.49 | 0.29 | 0.16 | 0.65 | | 0.64 | 0.04 | | 0.29 | [83] |
| 362 | OCCS | CCCCCC | 2.91 | 2.41 | 2.36 | 4.68 | | | | | 4.25 | [84] |

Continued on next page

**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 363 | OCCS | C1CCCCC1 | 2.50 | 2.18 | 1.99 | 4.15 | | | | | 3.55 | [84] |
| 364 | OCCS | CC1CCCC1 | 2.51 | 2.18 | 1.99 | 3.70 | | | | | 3.64 | [84] |
| 365 | OCCS | CCCCCCC | 3.25 | 2.70 | 2.67 | 5.14 | | | | | 4.51 | [84] |
| 366 | OCCS | CC1CCCCC1 | 2.80 | 2.50 | 2.30 | 4.38 | | | | | 3.89 | [84] |
| 367 | OCCS | CC(C)CC(C)(C)C | 3.23 | 3.00 | 3.01 | 5.59 | | | | | 4.61 | [84] |
| 368 | OCCS | c1ccccc1 | 0.96 | 1.00 | 0.70 | 2.04 | | | | | 1.82 | [84] |
| 369 | OCCS | Cc1ccccc1 | 1.29 | 1.59 | 1.24 | 2.23 | | | | | 2.19 | [84] |
| 370 | COCCO | CCCCCC | 2.37 | 1.97 | 1.99 | 2.69 | 2.82 | 2.75 | 3.04 | | 2.77 | [47 , 73] |
| 371 | COCCO | c1ccccc1 | 1.00 | 0.76 | 0.53 | 1.42 | 1.08 | 1.51 | 1.10 | | 1.19 | [73 , 47] |
| 372 | COCCO | C1CCCCC1 | 2.05 | 1.80 | 1.68 | 2.59 | 2.50 | 2.15 | 1.92 | | 2.33 | [85 , 85] |
| 373 | CC(C)CO | CCCCCC | 1.49 | 1.35 | 1.28 | 1.57 | 1.66 | 2.14 | 2.12 | 1.71 | 2.08 | [76] |
| 374 | CC(C)CO | CCCCCCC | 1.66 | 1.52 | 1.45 | 1.69 | 1.83 | 2.43 | 1.92 | 1.91 | 1.77 | [86] |
| 375 | CC(C)CO | c1ccccc1 | 0.95 | 1.05 | 0.76 | 1.18 | 1.24 | 1.24 | 0.44 | 1.10 | 1.65 | [77] |
| 376 | CCC(C)(C)O | C1CCCCC1 | 1.08 | 1.08 | 0.89 | 1.04 | 1.19 | 1.23 | 0.64 | | 1.34 | [87] |
| 377 | CC(C)(C)O | CCCCC | 1.37 | 1.15 | 1.08 | 1.00 | 1.30 | 1.55 | 1.86 | 1.44 | 1.25 | [61] |
| 378 | CC(C)(C)O | CCCCCC | 1.56 | 1.36 | 1.25 | 1.12 | 1.46 | 1.79 | 1.67 | 1.62 | 1.37 | [61 , 76] |
| 379 | CC(C)(C)O | C1CCCCC1 | 1.51 | 1.32 | 1.05 | 1.24 | 1.46 | 1.45 | 0.77 | 1.58 | 1.31 | [61] |
| 380 | CC(C)(C)O | CCCC(C)C | 1.75 | 1.36 | 1.25 | 1.12 | 1.47 | | | 1.62 | 1.38 | [61] |
| 381 | CC(C)(C)O | CCCCCCC | 1.93 | 1.54 | 1.41 | 1.24 | 1.61 | 2.04 | 1.49 | 1.79 | 1.56 | [61] |
| 382 | CC(C)(C)O | CCCCCCCC | 1.72 | 1.70 | 1.56 | 1.35 | 1.81 | 2.29 | 1.41 | 1.96 | 1.74 | [61 , 61] |
| 383 | CC(C)(C)O | CC(C)C(C)C(C)C | 2.11 | 1.71 | 1.56 | 1.35 | 1.50 | | | | 1.57 | [61] |
| 384 | CC(C)(C)O | CCC1CCCCC1 | 0.96 | 1.70 | 1.38 | 1.41 | | | | 1.94 | 1.64 | [61] |
| 385 | CC(C)(C)O | CCCCCCCCC | 1.17 | 1.86 | 1.71 | 1.47 | 2.09 | 2.55 | 1.32 | 2.13 | 1.96 | [61] |
| 386 | CC(C)(C)O | c1ccccc1 | 1.06 | 1.10 | 0.74 | 1.20 | 1.18 | 1.02 | 0.19 | 0.87 | 1.56 | [77] |
| 387 | CC(C)(C)O | Cc1ccccc1 | -0.15 | 1.25 | 0.82 | 1.27 | 1.25 | 1.16 | 0.33 | 1.03 | 1.40 | [61] |
| 388 | CC(C)(C)O | CC=C(C)C | 0.00 | 1.12 | 1.09 | 0.92 | | 0.67 | 1.60 | | 0.44 | [88] |
| 389 | CC(C)(C)O | CCO | -0.15 | 0.03 | 0.06 | 0.26 | 0.06 | -0.21 | 0.52 | -0.04 | -0.42 | [61] |
| 390 | CC(C)(C)O | C1COCCO1 | 0.00 | 0.89 | 0.85 | 1.11 | 0.21 | 0.41 | -0.16 | 0.75 | 0.49 | [61] |
| 391 | CC(C)(C)O | CCC(C)=O | 0.21 | 0.76 | 0.73 | 0.87 | 0.76 | 0.39 | 0.07 | 0.63 | 0.51 | [61] |
| 392 | CC(C)(C)O | CCN(CC)CC | 1.22 | 0.40 | 0.27 | -0.29 | -0.07 | 1.88 | 0.48 | 0.58 | 0.58 | [61] |
| 393 | C=C(CCC#N)C#N | CCCCCC | 3.88 | | | | | | | | 3.66 | [47] |
| 394 | C=C(CCC#N)C#N | C1CCCCC1 | 3.28 | | | | | | | | 3.12 | [47] |
| 395 | C=C(CCC#N)C#N | c1ccccc1 | 1.28 | | | | | | | | 0.95 | [47] |
| 396 | C=C(CCC#N)C#N | CC=C(C)C | 2.42 | | | | | | | | 2.42 | [47] |
| 397 | C=C(CCC#N)C#N | CC(=C)C=C | 1.68 | | | | | | | | 1.76 | [47] |
| 398 | CC(CCC#N)C#N | CCCCC | 3.25 | | | | | | | | 3.27 | [47] |
| 399 | CC(CCC#N)C#N | CCC(C)C | 3.13 | | | | | | | | 3.29 | [47] |
| 400 | CC(CCC#N)C#N | CCCCCC | 3.74 | | | | | | | | 3.64 | [47] |
| 401 | CC(CCC#N)C#N | C1CCCCC1 | 3.17 | | | | | | | | 3.00 | [47] |
| 402 | CC(CCC#N)C#N | c1ccccc1 | 1.18 | | | | | | | | 0.78 | [47] |
| 403 | CC(CCC#N)C#N | CC=C(C)C | 2.30 | | | | | | | | 2.30 | [47] |
| 404 | CC(CCC#N)C#N | CC(=C)C=C | 1.56 | | | | | | | | 1.58 | [47] |
| 405 | CC1CCC[S]1(=O)=O | CCCCCC | 3.25 | 2.70 | 2.64 | 3.56 | | 3.10 | 6.07 | | 2.89 | [47 , 73] |
| 406 | CC1CCC[S]1(=O)=O | c1ccccc1 | 0.85 | 0.51 | 0.54 | 0.72 | | 1.45 | 2.72 | | 0.41 | [47 , 73] |
| 407 | CC(C)[N+]([O-])=O | CCCCC | 1.70 | 1.02 | 1.02 | 1.55 | | 1.08 | 1.08 | 1.77 | 1.84 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 408 | CC(C)[N+]([O-])=O | CCCCCC | 1.93 | 1.15 | 1.17 | 1.68 | | 1.23 | 0.94 | 1.98 | 1.98 | [61] |
| 409 | CC(C)[N+]([O-])=O | C1CCCCC1 | 1.66 | 1.05 | 0.99 | 1.71 | | 0.92 | 0.29 | 1.87 | 1.68 | [61] |
| 410 | CC(C)[N+]([O-])=O | CCCCCCC | 2.16 | 1.26 | 1.31 | 1.81 | | 1.38 | 0.81 | 2.19 | 2.14 | [61] |
| 411 | CC(C)[N+]([O-])=O | CC1CCCCC1 | 1.85 | 1.18 | 1.13 | 1.74 | | 1.09 | 0.54 | 2.04 | 1.89 | [61] |
| 412 | CC(C)[N+]([O-])=O | CCCC=C | 1.02 | 0.80 | 0.80 | 1.00 | | 0.75 | 1.08 | 1.29 | 1.28 | [61] |
| 413 | CC(C)[N+]([O-])=O | CC(C)C=C | 1.02 | 0.80 | 0.80 | 1.00 | | | | | 1.21 | [61] |
| 414 | CC(C)[N+]([O-])=O | CC(=C)C=C | 0.55 | 0.68 | 0.68 | 0.41 | | | | | 0.73 | [61] |
| 415 | CC(C)[N+]([O-])=O | CO | 1.93 | 1.56 | 1.64 | 1.90 | | 0.34 | 2.66 | 2.52 | 2.09 | [61] |
| 416 | CC(C)[N+]([O-])=O | CCO | 2.02 | 1.66 | 1.56 | 1.92 | | 0.54 | 1.08 | 2.21 | 2.09 | [61] |
| 417 | CC(C)[N+]([O-])=O | CCCCl | 0.18 | 0.21 | 0.21 | 0.31 | | | | | 0.49 | [61] |
| 418 | CC(C)[N+]([O-])=O | ClCCl | -0.58 | -0.09 | -0.05 | -0.02 | | -0.08 | -0.29 | -0.17 | -0.09 | [61] |
| 419 | CC(C)[N+]([O-])=O | ClC(Cl)Cl | -0.36 | -0.76 | -0.76 | -0.42 | | 0.23 | | -0.15 | -0.13 | [61] |
| 420 | CC(C)[N+]([O-])=O | ClC(Cl)(Cl)Cl | 0.94 | 0.71 | 0.71 | 0.76 | | 0.82 | 0.05 | 1.00 | 0.86 | [61] |
| 421 | CC(C)[N+]([O-])=O | CCBr | -0.14 | 0.25 | 0.28 | 0.54 | | -0.16 | | | 0.42 | [61] |
| 422 | CC(C)[N+]([O-])=O | CCI | -0.06 | 0.72 | 0.72 | 0.76 | | | | | 0.78 | [61] |
| 423 | CC(C)[N+]([O-])=O | C(=S)=S | 0.96 | 1.12 | 1.13 | 1.18 | | 0.54 | -0.31 | | 1.37 | [61] |
| 424 | CCCC(C)=O | CCCCC | 1.04 | 0.97 | 0.97 | 1.13 | | 0.44 | 0.46 | 1.05 | 0.95 | [54 , 61] |
| 425 | CCCC(C)=O | CCCCCC | 1.20 | 1.12 | 1.12 | 1.23 | | 0.52 | 0.36 | 1.16 | 1.10 | [54 , 61] |
| 426 | CCCC(C)=O | C1CCCCC1 | 1.02 | 1.00 | 0.94 | 1.25 | | 0.34 | -0.09 | 1.08 | 1.03 | [54 , 61] |
| 427 | CCCC(C)=O | CCCC(C)C | 1.15 | 1.12 | 1.12 | 1.23 | | | | 1.19 | 1.08 | [54] |
| 428 | CCCC(C)=O | CCCCCCC | 1.35 | 1.25 | 1.26 | 1.33 | | 0.60 | 0.27 | 1.27 | 1.20 | [54 , 61] |
| 429 | CCCC(C)=O | CC(C)CC(C)C | 1.24 | 1.24 | 1.26 | 1.33 | | | | 1.32 | 1.17 | [54 , 61] |
| 430 | CCCC(C)=O | CCCCCCCC | 1.49 | 1.36 | 1.40 | 1.43 | | 0.69 | 0.24 | 1.38 | 1.31 | [54 , 61] |
| 431 | CCCC(C)=O | CC(C)C(C)C(C)C | 1.30 | 1.36 | 1.40 | 1.43 | | | | | 1.19 | [54 , 61] |
| 432 | CCCC(C)=O | CC(C)CCC(C)C | 1.40 | 1.36 | 1.40 | 1.43 | | | | | 1.25 | [54] |
| 433 | CCCC(C)=O | CCC1CCCCC1 | 1.28 | 1.28 | 1.23 | 1.40 | | | | 1.35 | 1.22 | [54 , 61] |
| 434 | CCCC(C)=O | CCCCCCCCC | 1.62 | 1.46 | 1.53 | 1.52 | | 0.77 | 0.20 | 1.49 | 1.46 | [54 , 61] |
| 435 | CC(C)O | CCCCC | 1.67 | 1.42 | 1.34 | 1.51 | 1.88 | 2.07 | 2.39 | 1.74 | 1.61 | [54 , 61 , 61] |
| 436 | CC(C)O | CCCCCC | 1.89 | 1.64 | 1.54 | 1.64 | 2.06 | 2.36 | 2.19 | 1.95 | 1.88 | [54] |
| 437 | CC(C)O | C1CCCCC1 | 1.67 | 1.58 | 1.30 | 1.62 | 1.98 | 1.87 | 1.26 | 1.98 | 1.60 | [54 , 61 , 61] |
| 438 | CC(C)O | CCCC(C)C | 1.82 | 1.64 | 1.54 | 1.64 | 2.06 | | | 1.93 | 1.85 | [54 , 61 , 61] |
| 439 | CC(C)O | CCCCCCC | 2.11 | 1.83 | 1.73 | 1.78 | 2.24 | 2.65 | 2.00 | 2.16 | 2.04 | [54 , 61 , 61 , 86] |
| 440 | CC(C)O | CC(C)CC(C)C | 1.96 | 1.83 | 1.73 | 1.78 | 2.21 | | | 2.10 | 2.01 | [54 , 61] |
| 441 | CC(C)O | CCCCCCCC | 2.32 | 2.01 | 1.91 | 1.91 | 2.46 | 2.95 | 1.91 | 2.36 | 2.24 | [54 , 61 , 61 , 61] |
| 442 | CC(C)O | CC(C)CC(C)(C)C | 2.06 | 1.99 | 1.94 | 1.91 | 2.30 | 3.11 | 2.66 | 2.25 | 2.01 | [54] |
| 443 | CC(C)O | CC(C)C(C)C(C)C | 2.06 | 2.01 | 1.91 | 1.91 | 2.14 | | | | 2.07 | [61 , 61] |
| 444 | CC(C)O | CC(C)CCC(C)C | 2.19 | 2.01 | 1.91 | 1.91 | | | | | 2.17 | [54] |
| 445 | CC(C)O | CCC1CCCCC1 | 2.05 | 1.99 | 1.69 | 1.81 | | | | 2.37 | 2.09 | [54 , 61 , 61] |
| 446 | CC(C)O | CCCCCCCCC | 2.52 | 2.17 | 2.09 | 2.04 | 2.76 | 3.25 | 1.82 | 2.57 | 2.38 | [54 , 61 , 61] |
| 447 | CC(C)O | CCC(C)CCC(C)C | 2.37 | 2.18 | 2.09 | 2.04 | | | | | 2.09 | [61] |
| 448 | CC(C)O | c1ccccc1 | 1.13 | 1.28 | 0.89 | 1.38 | 1.55 | 1.30 | 0.61 | 1.35 | 1.56 | [89 , 90] |
| 449 | CC(C)O | Cc1ccccc1 | 1.36 | 1.43 | 0.97 | 1.42 | 1.64 | 1.48 | 0.76 | 1.50 | 1.71 | [61 , 89] |
| 450 | CC(C)O | Cc1cccc(C)c1 | 1.52 | 1.50 | 1.01 | 1.48 | 1.80 | 1.54 | 0.80 | | 2.65 | [89] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 451 | CC(C)O | Cc1ccc(C)cc1 | 1.52 | 1.50 | 1.01 | 1.48 | 1.73 | 1.50 | 0.87 | 1.62 | 1.91 | [89] |
| 452 | CC(C)O | Cc1ccccc1C | 1.47 | 1.50 | 1.01 | 1.48 | 1.79 | 1.50 | 0.80 | | 2.31 | [89] |
| 453 | CC(C)O | CCO | -0.06 | 0.01 | 0.02 | 0.05 | 0.31 | -0.21 | 0.01 | -0.02 | -0.13 | [61] |
| 454 | CC(C)O | C1COCCO1 | 0.09 | 0.94 | 0.91 | 1.16 | 0.47 | 0.55 | 0.11 | 1.10 | 1.10 | [61] |
| 455 | CC(C)O | CCC(C)=O | 0.20 | 0.82 | 0.77 | 0.84 | 1.10 | 0.58 | 0.45 | 0.92 | 0.89 | [61] |
| 456 | CCCOCCO | CCCCCC | 1.50 | 1.36 | 1.36 | 1.70 | 1.64 | 1.92 | 2.67 | | 1.63 | [83] |
| 457 | CCCOCCO | C1CCCCC1 | 1.28 | 1.21 | 1.14 | 1.57 | 1.39 | 1.46 | 1.42 | | 1.35 | [83] |
| 458 | CCCOCCO | CC1CCCC1 | 1.28 | 1.21 | 1.14 | 1.37 | 1.29 | | | | 1.52 | [83] |
| 459 | CCCOCCO | CCCCCCC | 1.69 | 1.54 | 1.54 | 1.86 | 1.80 | 2.17 | 2.42 | | 1.81 | [83] |
| 460 | CCCOCCO | CCCCCCCCC | 2.06 | 1.86 | 1.89 | 2.19 | 2.29 | 2.69 | 2.18 | | 2.16 | [83] |
| 461 | CCCOCCO | c1ccccc1 | 0.54 | 0.42 | 0.30 | 0.85 | 0.62 | 0.97 | 0.56 | | 0.48 | [83] |
| 462 | CCCOCCO | Cc1ccccc1 | 0.77 | 0.72 | 0.55 | 0.96 | 0.70 | 1.08 | 0.75 | | 0.71 | [83] |
| 463 | CCCOCCO | Cc1cccc(C)c1 | 0.91 | 0.95 | 0.76 | 1.08 | 0.86 | 1.16 | 0.82 | | 1.00 | [83] |
| 464 | CCCOCCO | Cc1ccc(C)cc1 | 0.92 | 0.95 | 0.76 | 1.08 | 0.80 | 1.13 | 0.90 | | 0.95 | [83] |
| 465 | CCCOCCO | Cc1ccccc1C | 0.86 | 0.95 | 0.76 | 1.08 | 0.80 | 1.12 | 0.82 | | 0.92 | [83] |
| 466 | CCCOCCO | CCc1ccccc1 | 0.91 | 0.88 | 0.70 | 1.24 | 0.89 | 1.48 | 0.92 | | 0.94 | [83] |
| 467 | CCCOCCO | C=CCCCCC=C | 1.14 | 1.64 | 1.63 | 1.55 | | | | | 1.25 | [83] |
| 468 | CCCOCCO | CCCCCC#C | 0.43 | 0.14 | 0.15 | 1.08 | | | | | 0.81 | [83] |
| 469 | CCCOCCO | CC(C)O | 0.11 | 0.46 | 0.41 | -0.05 | 0.62 | -0.25 | -0.29 | | 0.39 | [83] |
| 470 | CCCOCCO | C1CCOC1 | -0.29 | 0.16 | 0.16 | 0.77 | -0.11 | -0.09 | 0.20 | | 0.03 | [83] |
| 471 | CCCOCCO | C1COCCO1 | 0.07 | 0.11 | -0.07 | 0.53 | 0.04 | 0.33 | -0.04 | | 0.42 | [83] |
| 472 | CCCOCCO | CCC(C)=O | 0.17 | 0.73 | 0.75 | 0.52 | 0.57 | 0.12 | 0.36 | | 0.43 | [83] |
| 473 | CCCOCCO | ClCCl | -0.56 | -0.21 | -0.12 | -0.20 | -0.33 | -0.08 | -0.08 | | -0.36 | [83] |
| 474 | CCCOCCO | CC(Cl)CCl | 0.26 | -0.33 | -0.33 | 0.89 | 0.63 | | | | 0.38 | [83] |
| 475 | CCCOCCO | Clc1ccccc1 | 0.55 | 0.75 | 0.55 | 0.62 | 0.65 | 0.92 | 0.24 | | 0.48 | [83] |
| 476 | CCCOCCO | Brc1ccccc1 | 1.07 | 0.49 | 0.29 | 1.15 | 0.74 | 0.90 | -0.15 | | 0.58 | [83] |
| 477 | CCCOCCO | CC#N | 0.93 | 0.84 | 0.97 | 0.76 | 0.79 | -0.01 | -0.34 | | 0.78 | [83] |
| 478 | CCCOCCO | Fc1ccccc1 | 0.49 | 0.29 | 0.16 | 0.65 | | 0.69 | 0.16 | | 0.34 | [83] |
| 479 | Cc1cncc(C)c1 | CCCCCC | 1.07 | 0.70 | 0.45 | 0.41 | | | | | 0.57 | [75] |
| 480 | Cc1cncc(C)c1 | CCCCCCC | 1.19 | 0.76 | 0.51 | 0.28 | | | | | 1.11 | [75] |
| 481 | Cc1cncc(C)c1 | CCCCCCCC | 1.30 | 0.80 | 0.56 | 0.14 | | | | | 1.37 | [75] |
| 482 | CCC#CCC | CCCCCCCC | 0.29 | 0.17 | 0.20 | 0.34 | | | | | 0.35 | [82] |
| 483 | CC(C)CCO | CCCCC | 1.16 | 0.94 | 0.93 | 1.24 | 1.25 | 1.29 | 1.85 | | 0.54 | [61 , 61] |
| 484 | CC(C)CCO | CCCCCC | 1.33 | 1.13 | 1.09 | 1.35 | 1.38 | 1.49 | 1.64 | | 1.39 | [61 , 91] |
| 485 | CC(C)CCO | C1CCCCC1 | 1.15 | 1.05 | 0.91 | 1.25 | 1.34 | 1.13 | 0.69 | | 1.11 | [61] |
| 486 | CC(C)CCO | CCCC(C)C | 1.28 | 1.13 | 1.09 | 1.35 | 1.40 | | | | 1.25 | [61] |
| 487 | CC(C)CCO | CCCCCCC | 1.49 | 1.29 | 1.24 | 1.46 | 1.51 | 1.69 | 1.45 | | 1.44 | [61] |
| 488 | CC(C)CCO | CC(C)CC(C)C | 1.39 | 1.29 | 1.23 | 1.46 | 1.51 | | | | 1.39 | [61] |
| 489 | CC(C)CCO | CCCCCCCC | 1.64 | 1.44 | 1.38 | 1.56 | 1.68 | 1.90 | 1.36 | | 1.59 | [61 , 61] |
| 490 | CC(C)CCO | CC(C)C(C)C(C)C | 1.46 | 1.44 | 1.37 | 1.56 | 1.38 | | | | 1.47 | [61] |
| 491 | CC(C)CCO | CCCCCCCCC | 1.79 | 1.57 | 1.51 | 1.67 | 1.93 | 2.11 | 1.28 | | 1.84 | [61] |
| 492 | CC(C)CCO | CCC(C)CCC(C)C | 1.69 | 1.58 | 1.51 | 1.67 | | | | | 1.52 | [61] |
| 493 | CC(C)CCO | Cc1ccccc1 | 1.00 | 1.00 | 0.73 | 1.03 | 1.15 | 0.84 | 0.23 | | 1.09 | [61] |
| 494 | CC(C)CCO | CCO | 0.12 | 0.07 | 0.09 | 0.09 | 0.27 | -0.22 | 0.80 | | -0.13 | [61] |
| 495 | CC(C)CCO | C1COCCO1 | 0.14 | 0.90 | 0.82 | 0.97 | 0.10 | 0.19 | -0.24 | | 0.74 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 496 | CC(C)CCO | CCC(C)=O | 0.13 | 0.68 | 0.70 | 0.82 | 0.75 | 0.20 | -0.03 | | 0.60 | [61] |
| 497 | CC(C)CCO | CCN(CC)CC | -0.16 | 0.21 | 0.15 | 0.00 | -0.40 | 1.46 | 0.39 | | -0.42 | [61] |
| 498 | CC1CC[S](=O)(=O)C1 | CCCCCC | 3.25 | 2.70 | 2.64 | 3.56 | | | | | 3.39 | [84] |
| 499 | CC1CC[S](=O)(=O)C1 | C1CCCCC1 | 2.75 | 2.21 | 2.22 | 3.04 | | | | | 2.83 | [84] |
| 500 | CC1CC[S](=O)(=O)C1 | CC1CCCC1 | 2.78 | 2.21 | 2.21 | 2.73 | | | | | 2.84 | [84] |
| 501 | CC1CC[S](=O)(=O)C1 | CCCCCCC | 3.66 | 3.06 | 3.01 | 3.92 | | | | | 3.67 | [84] |
| 502 | CC1CC[S](=O)(=O)C1 | CC1CCCCC1 | 3.11 | 2.59 | 2.59 | 3.24 | | | | | 3.11 | [84] |
| 503 | CC1CC[S](=O)(=O)C1 | CC(C)CC(C)(C)C | 3.67 | 3.48 | 3.42 | 4.27 | | | | | 3.74 | [84] |
| 504 | CC1CC[S](=O)(=O)C1 | c1ccccc1 | 0.85 | 0.51 | 0.54 | 0.72 | | | | | 0.53 | [84] |
| 505 | CC1CC[S](=O)(=O)C1 | Cc1ccccc1 | 1.29 | 0.94 | 0.93 | 1.00 | | | | | 0.83 | [84] |
| 506 | CCC(=O)CC | CCCCC | 0.97 | 0.69 | 0.69 | 0.85 | | 0.43 | 0.35 | | 0.94 | [74] |
| 507 | CCC(=O)CC | CCCC=C | 0.49 | 0.39 | 0.39 | 0.48 | | 0.17 | 0.34 | | 0.58 | [74] |
| 508 | CC(=O)CC(C)(C)O | CCCCCC | 1.96 | 1.91 | 1.88 | 2.18 | | 1.30 | 1.57 | | 2.04 | [92] |
| 509 | CC(=O)O | CCCCC | 3.46 | 2.26 | 2.31 | 2.08 | 2.65 | 1.64 | 0.82 | 2.66 | 2.46 | [54] |
| 510 | CC(=O)O | CCCCCC | 3.91 | 2.54 | 2.64 | 2.37 | 2.94 | 1.89 | 0.72 | 2.91 | 2.79 | [54] |
| 511 | CC(=O)O | C1CCCCC1 | 3.40 | 2.33 | 2.24 | 2.60 | 2.81 | 1.64 | 0.27 | 2.66 | 2.88 | [54 , 93] |
| 512 | CC(=O)O | CCCC(C)C | 3.78 | 2.54 | 2.64 | 2.37 | 2.91 | | | 2.94 | 2.78 | [54] |
| 513 | CC(=O)O | CCCCCCC | 4.35 | 2.79 | 2.97 | 2.66 | 3.22 | 2.16 | 0.62 | 3.16 | 3.14 | [54 , 93] |
| 514 | CC(=O)O | CC(C)CC(C)C | 4.06 | 2.79 | 2.96 | 2.66 | 3.12 | | | 3.22 | 2.96 | [54] |
| 515 | CC(=O)O | CCCCCCCC | 4.79 | 3.03 | 3.29 | 2.95 | 3.55 | 2.42 | 0.58 | 3.42 | 3.37 | [54] |
| 516 | CC(=O)O | CC(C)C(C)C(C)C | 4.25 | 3.03 | 3.28 | 2.95 | 3.19 | | | | 3.06 | [54] |
| 517 | CC(=O)O | CC(C)CCC(C)C | 4.53 | 3.03 | 3.28 | 2.95 | | | | | 3.25 | [54] |
| 518 | CC(=O)O | CCC1CCCCC1 | 4.17 | 2.86 | 2.89 | 3.04 | | | | 3.23 | 3.12 | [54] |
| 519 | CC(=O)O | CCCCCCCCC | 5.22 | 3.25 | 3.61 | 3.25 | 3.96 | 2.69 | 0.54 | 3.67 | 3.63 | [54] |
| 520 | CC(=O)O | c1ccccc1 | 1.94 | 1.12 | 0.84 | 1.35 | 1.46 | 1.28 | 0.01 | 1.45 | 1.34 | [93] |
| 521 | CC(C)=O | CCCCCC | 2.21 | 1.74 | 1.81 | 1.81 | 1.60 | 1.17 | 0.78 | 1.89 | 1.81 | [47 , 54 , 61 , 61 , 73 , 94] |
| 522 | CC(C)=O | c1ccccc1 | 0.51 | 0.55 | 0.34 | 0.34 | 0.29 | 0.75 | -0.05 | 0.51 | 0.51 | [47 , 61 , 61 , 47 , 96] |
| 523 | CC(C)=O | CCCCC | 1.94 | 1.56 | 1.59 | 1.66 | 1.39 | 1.02 | 0.89 | 1.68 | 1.65 | [54 , 61 , 61 , 74] |
| 524 | CC(C)=O | C1CCCCC1 | 1.92 | 1.60 | 1.54 | 1.84 | 1.34 | 0.94 | 0.25 | 1.98 | 1.84 | [54 , 61 , 61] |
| 525 | CC(C)=O | CCCC(C)C | 2.13 | 1.74 | 1.81 | 1.81 | 1.60 | | | 1.85 | 1.88 | [54 , 61 , 61] |
| 526 | CC(C)=O | CCCCCCC | 2.47 | 1.89 | 2.03 | 1.96 | 1.80 | 1.32 | 0.67 | 2.10 | 2.12 | [54 , 61 , 61 , 94] |
| 527 | CC(C)=O | CC(C)CC(C)C | 2.29 | 1.89 | 2.03 | 1.96 | 1.75 | | | 2.01 | 2.04 | [54 , 61] |
| 528 | CC(C)=O | CCCCCCCC | 2.72 | 2.04 | 2.24 | 2.12 | 2.04 | 1.48 | 0.62 | 2.29 | 2.35 | [54 , 61 , 61 , 61 , 95 , 94] |
| 529 | CC(C)=O | CC(C)C(C)C(C)C | 2.41 | 2.04 | 2.24 | 2.12 | 1.71 | | | | 2.14 | [54 , 61 , 61] |
| 530 | CC(C)=O | CC(C)CCC(C)C | 2.57 | 2.04 | 2.24 | 2.12 | | | | | 2.24 | [54] |
| 531 | CC(C)=O | CCC1CCCCC1 | 2.38 | 1.94 | 1.97 | 2.06 | | | | 2.34 | 2.21 | [54 , 61 , 61] |
| 532 | CC(C)=O | CCCCCCCCC | 2.97 | 2.17 | 2.45 | 2.27 | 2.37 | 1.65 | 0.58 | 2.50 | 2.54 | [54 , 61 , 61] |
| 533 | CC(C)=O | CCC(C)CCC(C)C | 2.80 | 2.17 | 2.44 | 2.27 | | | | | 2.16 | [61] |
| 534 | CC(C)=O | Cc1ccccc1 | 1.22 | 0.69 | 0.49 | 0.54 | 0.41 | 0.73 | 0.02 | 0.68 | 0.64 | [61] |
| 535 | CC(C)=O | CCCC=C | 1.22 | 1.12 | 1.13 | 1.10 | 1.17 | 0.56 | 0.89 | 1.24 | 1.15 | [74] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 536 | CC(C)=O | CO | 0.20 | 0.67 | 0.72 | 0.74 | 0.63 | 0.19 | 2.18 | 1.10 | 0.61 | [96 , 61] |
| 537 | CC(C)=O | CCO | 0.45 | 0.86 | 0.79 | 0.83 | 0.83 | 0.29 | 0.89 | 0.81 | 0.85 | [96 , 61 , 95] |
| 538 | CC(C)=O | C1COCCO1 | 0.15 | 0.38 | 0.27 | 0.43 | -0.15 | 0.48 | -0.16 | 0.46 | 0.28 | [61 , 95] |
| 539 | CC(C)=O | CCC(C)=O | 0.04 | 0.01 | 0.02 | 0.02 | 0.24 | -0.12 | -0.11 | 0.16 | 0.06 | [61 , 95] |
| 540 | CC(C)=O | ClC(Cl)Cl | -0.40 | -0.84 | -0.89 | -0.92 | -0.89 | 0.20 |  | -1.05 | -0.71 | [61] |
| 541 | CC(C)=O | ClC(Cl)(Cl)Cl | -0.40 | 0.74 | 0.74 | 0.72 | 0.48 | 0.87 | 0.05 | 0.86 | 0.86 | [61 , 95] |
| 542 | CC(C)=O | CCI | 0.09 | 0.61 | 0.58 | 0.62 | 0.87 |  |  |  | 0.82 | [61] |
| 543 | CC(C)=O | CCN(CC)CC | 1.44 | 1.24 | 1.36 | 1.41 | 1.31 | 1.24 | 0.10 | 1.46 | 1.42 | [61] |
| 544 | CC(C)=O | C(=S)=S | 1.34 | 1.46 | 1.41 | 1.44 |  | 0.66 | -0.25 |  | 1.48 | [61] |
| 545 | CC#N | CCCCC | 3.68 | 2.85 | 3.01 | 3.02 | 2.88 | 2.47 | 1.97 | 3.04 | 2.96 | [97 , 54 , 61 , 61 , 98 , 98 , 99 , 100 , 100 , 100 , 100] |
| 546 | CC#N | C1CCCC1 | 3.17 | 2.49 | 2.47 | 2.73 | 2.62 | 1.89 | 1.20 | 2.88 | 2.75 | [97 , 61] |
| 547 | CC#N | CCC(C)C | 3.54 | 2.84 | 3.01 | 3.02 |  | 2.57 | 2.32 |  | 2.76 | [97 , 61] |
| 548 | CC#N | CCCCCC | 4.18 | 3.18 | 3.45 | 3.26 | 3.24 | 2.81 | 1.82 | 3.39 | 3.27 | [97 , 54 , 61 , 61 , 98 , 98 , 98 , 47 , 99 , 73 , 100 , 100 , 100] |
| 549 | CC#N | C1CCCCC1 | 3.61 | 2.85 | 2.91 | 3.19 | 3.04 | 2.34 | 1.12 | 3.26 | 3.08 | [97 , 54 , 61 , 61 , 98 , 98 , 99] |
| 550 | CC#N | CCCC(C)C | 4.04 | 3.18 | 3.44 | 3.26 | 3.18 |  |  | 3.36 | 3.22 | [97 , 54 , 61 , 61 , 61 , 99] |
| 551 | CC#N | CCC(C)CC | 3.99 | 3.18 | 3.44 | 3.26 | 3.16 |  |  |  | 3.17 | [97 , 99] |
| 552 | CC#N | CC(C)C(C)C | 3.85 | 3.18 | 3.44 | 3.26 | 3.09 |  |  | 3.33 | 3.27 | [97 , 61] |
| 553 | CC#N | CCC(C)(C)C | 3.83 | 3.23 | 3.52 | 3.25 | 3.03 |  |  |  | 3.12 | [97 , 61 , 99] |
| 554 | CC#N | CCCCCCC | 4.66 | 3.49 | 3.88 | 3.50 | 3.58 | 3.16 | 1.67 | 3.74 | 3.63 | [97 , 54 , 61 , 61 , 98 , 98 , 99 , 100 , 100 , 100 , 100] |
| 555 | CC#N | CCCC(C)CC | 4.48 | 3.49 | 3.87 | 3.50 |  |  |  |  | 3.70 | [97] |
| 556 | CC#N | CCCC(C)(C)C | 4.31 | 3.54 | 3.95 | 3.49 | 5.04 |  |  |  | 3.56 | [97 , 61] |
| 557 | CC#N | CC(C)CC(C)C | 4.36 | 3.49 | 3.87 | 3.50 | 3.43 |  |  | 3.67 | 3.57 | [97 , 54 , 61] |
| 558 | CC#N | CCC(CC)CC | 4.33 | 3.49 | 3.87 | 3.50 |  |  |  |  | 3.61 | [97 , 61] |
| 559 | CC#N | CC1CCCCC1 | 4.02 | 3.18 | 3.34 | 3.26 | 3.30 | 2.66 | 1.39 | 3.53 | 3.47 | [97] |
| 560 | CC#N | CCCCCCCC | 5.14 | 3.79 | 4.30 | 3.74 | 3.98 | 3.52 | 1.60 | 4.07 | 4.00 | [97 , 54 , 61 , 61 , 61 , 98 , 98 , 99] |
| 561 | CC#N | CC(C)CC(C)(C)C | 4.63 | 3.83 | 4.37 | 3.74 | 3.62 | 3.63 | 2.17 | 3.95 | 3.68 | [97 , 61 , 99] |
| 562 | CC#N | CCC1CCCCC1 | 4.47 | 3.49 | 3.77 | 3.52 |  |  |  | 3.95 | 3.71 | [97 , 54 , 61 , 61] |
| 563 | CC#N | CCCCCCCCC | 5.61 | 4.08 | 4.73 | 3.99 | 4.45 | 3.88 | 1.54 | 4.42 | 4.40 | [97 , 54 , 61 , 61 , 98] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 564 | CC#N | c1ccccc1 | 1.62 | 1.13 | 0.97 | 1.07 | 1.25 | 1.95 | 0.62 | 1.27 | 1.07 | [97 , 101 , 47 , 73 , 100 , 100 , 100 , 100 , 100 , 102] |
| 565 | CC#N | Cc1ccccc1 | 2.06 | 1.38 | 1.29 | 1.36 | 1.53 | 2.00 | 0.73 | 1.55 | 1.47 | [97 , 61 , 100 , 100 , 100] |
| 566 | CC#N | Cc1cccc(C)c1 | 2.46 | 1.57 | 1.56 | 1.66 | 1.89 | 2.36 | 0.76 | | 1.89 | [97 , 100] |
| 567 | CC#N | Cc1ccc(C)cc1 | 2.50 | 1.57 | 1.56 | 1.66 | 1.82 | 2.31 | 0.81 | 1.75 | 1.89 | [97 , 100] |
| 568 | CC#N | Cc1ccccc1C | 2.34 | 1.57 | 1.56 | 1.66 | 1.79 | 2.30 | 0.76 | | 1.81 | [97 , 100] |
| 569 | CC#N | CCc1ccccc1 | 2.46 | 1.77 | 1.77 | 1.85 | 1.92 | 2.54 | 0.82 | 1.86 | 1.80 | [97 , 100 , 100 , 100] |
| 570 | CC#N | CCCC=C | 2.69 | 2.12 | 2.24 | 2.19 | 2.46 | 1.84 | 1.98 | 2.33 | 2.03 | [97 , 99] |
| 571 | CC#N | CCC(C)C=C | 3.13 | 2.45 | 2.67 | 2.45 | | | | | 2.62 | [97 , 61] |
| 572 | CC#N | CCCCC=C | 3.19 | 2.45 | 2.67 | 2.45 | 2.79 | 2.42 | 1.88 | 2.81 | 2.60 | [97 , 99] |
| 573 | CC#N | C1CCC=CC1 | 2.74 | 2.27 | 2.29 | 2.12 | 2.51 | 1.79 | 0.78 | | 2.49 | [97 , 99] |
| 574 | CC#N | CCCCCC=C | 3.63 | 2.77 | 3.10 | 2.70 | 3.08 | 2.50 | 1.68 | | 3.04 | [97 , 99] |
| 575 | CC#N | CCCCCCC=C | 4.17 | 3.06 | 3.52 | 2.95 | 3.48 | 2.73 | 1.59 | 3.22 | 3.37 | [97] |
| 576 | CC#N | CC1CCCC1 | 3.99 | 2.85 | 2.91 | 2.81 | 2.83 | | | 3.21 | 3.13 | [61] |
| 577 | CC#N | CCCCC(C)C | 4.53 | 3.49 | 3.87 | 3.50 | | | | | 3.55 | [61 , 99] |
| 578 | CC#N | CCC(C)C(C)C | 4.28 | 3.49 | 3.87 | 3.50 | | | | | 3.14 | [99] |
| 579 | CC#N | CC(C)C(C)C(C)C | 4.58 | 3.79 | 4.29 | 3.74 | 3.59 | | | | 3.65 | [54 , 61 , 61] |
| 580 | CC#N | CC(C)CCC(C)C | 4.89 | 3.79 | 4.29 | 3.74 | | | | | 3.85 | [54] |
| 581 | CC#N | CCC(C)CCC(C)C | 5.61 | 4.07 | 4.72 | 3.99 | | | | | 3.71 | [61] |
| 582 | CC#N | CCO | 1.85 | 0.92 | 0.90 | 1.37 | 1.91 | 0.76 | -0.06 | 1.46 | 1.38 | [61 , 100] |
| 583 | CC#N | CCCO | 2.25 | 1.02 | 1.12 | 1.44 | 2.00 | 1.04 | -0.12 | 1.80 | 1.87 | [100] |
| 584 | CC#N | CC(C)O | 1.84 | 1.02 | 1.11 | 1.53 | 2.12 | 1.04 | -0.11 | 1.68 | 1.61 | [100] |
| 585 | CC#N | CCCCO | 2.44 | 1.15 | 1.36 | 1.54 | 2.17 | 1.28 | -0.06 | 1.87 | 2.10 | [100] |
| 586 | CC#N | Cc1ccccc1O | -0.94 | -0.05 | -0.11 | -0.87 | | | | | 0.95 | [100] |
| 587 | CC#N | Cc1cccc(O)c1 | -0.65 | -0.05 | -0.11 | -0.87 | | 1.46 | -0.02 | -1.14 | 1.26 | [100] |
| 588 | CC#N | Cc1ccc(O)cc1 | -0.49 | -0.05 | -0.11 | -0.87 | | | | | 1.57 | [100] |
| 589 | CC#N | C1COCCO1 | 0.49 | 0.44 | 0.45 | 0.78 | -0.16 | 1.55 | 0.22 | 0.66 | 0.31 | [61] |
| 590 | CC#N | CC(C)=O | 0.04 | -0.05 | -0.02 | 0.10 | 0.09 | 0.14 | 0.28 | 0.16 | 0.04 | [99] |
| 591 | CC#N | CCC(C)=O | 0.39 | 0.11 | 0.21 | 0.20 | 0.17 | 0.36 | 0.49 | 0.39 | 0.20 | [61] |
| 592 | CC#N | ClCCl | -0.26 | 0.12 | 0.12 | 0.15 | 0.07 | 0.51 | 0.21 | 0.44 | -0.04 | [61] |
| 593 | CC#N | ClC(Cl)Cl | 0.09 | 0.35 | 0.36 | 0.21 | 0.39 | 1.09 | | 0.49 | 0.25 | [99] |
| 594 | CC(=O)c1ccccc1 | CCCCCC | 1.57 | 1.50 | 1.38 | 2.24 | 1.79 | 1.22 | 2.09 | 1.40 | 1.83 | [59 , 59 , 54 , 61 , 61 , 103 , 103 , 47] |
| 595 | CC(=O)c1ccccc1 | c1ccccc1 | 0.13 | 0.11 | 0.15 | 0.20 | 0.15 | 0.17 | 0.24 | -0.02 | 0.19 | [59 , 59 , 47] |
| 596 | CC(=O)c1ccccc1 | CCCCC | 1.38 | 1.29 | 1.18 | 2.04 | 1.58 | 1.14 | 2.32 | 1.30 | 1.68 | [54 , 61 , 61 , 103 , 74] |
| 597 | CC(=O)c1ccccc1 | C1CCCCC1 | 1.26 | 1.17 | 1.16 | 2.01 | 1.39 | 0.55 | 0.97 | 1.03 | 1.48 | [54 , 61 , 61 , 47] |
| 598 | CC(=O)c1ccccc1 | CCCC(C)C | 1.52 | 1.49 | 1.38 | 2.24 | 1.79 | | | 1.51 | 1.84 | [54 , 61 , 61] |
| 599 | CC(=O)c1ccccc1 | CCCCCCC | 1.75 | 1.68 | 1.58 | 2.43 | 1.99 | 1.29 | 1.86 | 1.51 | 1.94 | [54 , 61 , 61 , 103] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 600 | CC(=O)c1ccccc1 | CC(C)CC(C)C | 1.64 | 1.68 | 1.57 | 2.43 | 1.95 | | | 1.72 | 2.03 | [54 , 61 , 61] |
| 601 | CC(=O)c1ccccc1 | CC1CCCCC1 | 1.43 | 1.37 | 1.36 | 2.10 | 1.54 | 0.85 | 1.40 | 1.25 | 1.51 | [61] |
| 602 | CC(=O)c1ccccc1 | CCCCCCCC | 1.92 | 1.85 | 1.76 | 2.62 | 2.24 | 1.40 | 1.75 | 1.62 | 2.08 | [54 , 61 , 61 , 61] |
| 603 | CC(=O)c1ccccc1 | CC(C)C(C)C(C)C | 1.70 | 1.84 | 1.76 | 2.62 | 1.91 | | | | 2.01 | [54 , 61 , 61] |
| 604 | CC(=O)c1ccccc1 | CC(C)CCC(C)C | 1.82 | 1.85 | 1.76 | 2.62 | | | | | 2.24 | [61] |
| 605 | CC(=O)c1ccccc1 | CCC1CCCCC1 | 1.59 | 1.56 | 1.55 | 2.30 | | | | 1.39 | 1.77 | [54 , 61 , 61] |
| 606 | CC(=O)c1ccccc1 | CCCCCCCCC | 2.09 | 2.01 | 1.94 | 2.81 | 2.57 | 1.50 | 1.65 | 1.72 | 2.26 | [54 , 61 , 61] |
| 607 | CC(=O)c1ccccc1 | CCC(C)CCC(C)C | 1.98 | 2.00 | 1.94 | 2.81 | | | | | 2.07 | [61] |
| 608 | CC(=O)c1ccccc1 | Cc1ccccc1 | 0.31 | 0.31 | 0.31 | 0.39 | 0.28 | 0.20 | 0.41 | 0.10 | 0.23 | [61] |
| 609 | CC(=O)c1ccccc1 | CCCC=C | 0.79 | 0.91 | 0.82 | 1.42 | 1.26 | 0.99 | 2.33 | 0.95 | 1.30 | [61 , 74] |
| 610 | CC(=O)c1ccccc1 | CC=C(C)C | 0.80 | 1.13 | 0.96 | 1.55 | | 0.78 | 2.00 | | 1.12 | [47] |
| 611 | CC(=O)c1ccccc1 | CC(C)C=C | 0.81 | 0.90 | 0.82 | 1.42 | | | | | 1.02 | [61] |
| 612 | CC(=O)c1ccccc1 | CC(=C)C=C | 0.43 | 0.64 | 0.59 | 0.69 | 0.79 | | | | 0.68 | [61 , 47] |
| 613 | CC(=O)CC(C)=O | CCCCCC | | 2.75 | 2.75 | 3.22 | | | | | 1.43 | [104] |
| 614 | CC(=O)CC(C)=O | C1CCCCC1 | | 2.38 | 2.32 | 3.07 | | | | | 1.37 | [105] |
| 615 | CC(=O)CC(C)=O | c1ccccc1 | | 1.00 | 0.87 | 0.63 | | | | | 0.22 | [104 , 105] |
| 616 | CC(=O)CC(C)=O | Cc1ccccc1 | | 1.57 | 1.41 | 0.94 | | | | | 0.31 | [104 , 105] |
| 617 | CC(=O)N1CCCCC1 | CCCCC | | 0.80 | 0.78 | 1.17 | | | | | 1.77 | [74] |
| 618 | CC(=O)N1CCCCC1 | CCCC=C | | 0.48 | 0.47 | 0.80 | | | | | 1.24 | [74] |
| 619 | Nc1ccccc1 | CCCCCC | 2.42 | 2.31 | 2.19 | 3.04 | 2.94 | 1.55 | 1.29 | 3.11 | 3.21 | [59 , 59 , 59 , 59 , 47] |
| 620 | Nc1ccccc1 | c1ccccc1 | 0.51 | 0.57 | 0.57 | 0.67 | 0.98 | 0.32 | 0.05 | 0.74 | 0.78 | [59 , 59 , 59 , 59 , 61 , 47] |
| 621 | Nc1ccccc1 | CCCCC | 2.14 | 2.03 | 1.89 | 2.78 | 2.70 | 1.44 | 1.46 | 2.86 | 2.68 | [61] |
| 622 | Nc1ccccc1 | C1CCCCC1 | 2.01 | 1.86 | 1.84 | 2.54 | 2.64 | 0.85 | 0.52 | 2.50 | 2.46 | [61 , 61 , 47] |
| 623 | Nc1ccccc1 | CCCC(C)C | 2.35 | 2.31 | 2.18 | 3.04 | 2.93 | | | 3.24 | 3.02 | [61] |
| 624 | Nc1ccccc1 | CCCCCCC | 2.70 | 2.58 | 2.48 | 3.30 | 3.17 | 1.65 | 1.13 | 3.40 | 3.29 | [61] |
| 625 | Nc1ccccc1 | CC(C)CC(C)C | 2.53 | 2.57 | 2.47 | 3.30 | 3.10 | | | 3.64 | 3.32 | [61] |
| 626 | Nc1ccccc1 | CC1CCCCC1 | 2.26 | 2.14 | 2.14 | 2.69 | 2.79 | 1.09 | 0.82 | 2.92 | 2.82 | [61] |
| 627 | Nc1ccccc1 | CCCCCCCC | 2.97 | 2.83 | 2.76 | 3.56 | 3.44 | 1.79 | 1.07 | 3.68 | 3.60 | [61 , 61] |
| 628 | Nc1ccccc1 | CC(C)CC(C)(C)C | 2.70 | 2.91 | 2.80 | 3.56 | 3.22 | 2.34 | 1.72 | 4.04 | 3.61 | [61] |
| 629 | Nc1ccccc1 | CC(C)C(C)C(C)C | 2.63 | 2.81 | 2.75 | 3.56 | 3.10 | | | | 3.40 | [61] |
| 630 | Nc1ccccc1 | CCC1CCCCC1 | 2.50 | 2.41 | 2.42 | 2.97 | | | | 3.24 | 2.98 | [61] |
| 631 | Nc1ccccc1 | CCCCCCCCC | 3.23 | 3.06 | 3.04 | 3.82 | 3.79 | 1.92 | 1.00 | 3.96 | 3.90 | [61] |
| 632 | Nc1ccccc1 | CCC(C)CCC(C)C | 3.05 | 3.05 | 3.03 | 3.82 | | | | | 3.55 | [61] |
| 633 | Nc1ccccc1 | Cc1ccccc1 | 0.76 | 0.89 | 0.89 | 0.90 | 1.13 | 0.41 | 0.16 | 1.05 | 1.04 | [61] |
| 634 | Nc1ccccc1 | CCCC=C | 1.41 | 1.75 | 1.63 | 2.27 | 2.22 | 1.01 | 1.46 | 2.23 | 2.30 | [61] |
| 635 | Nc1ccccc1 | CC=C(C)C | 1.41 | 1.95 | 1.73 | 2.33 | | 0.83 | 1.23 | | 2.20 | [47] |
| 636 | Nc1ccccc1 | CC(C)C=C | 1.40 | 1.75 | 1.63 | 2.27 | | | | | 2.12 | [61] |
| 637 | Nc1ccccc1 | CC(=C)C=C | 0.90 | 1.50 | 1.40 | 1.46 | 1.70 | | | | 1.61 | [61 , 47] |
| 638 | Nc1ccccc1 | CO | 0.69 | 0.64 | 0.57 | 0.81 | 0.88 | 0.18 | 2.17 | 1.17 | 0.86 | [61] |
| 639 | Nc1ccccc1 | CCO | 0.55 | 0.49 | 0.05 | 1.05 | 1.00 | 0.20 | 0.75 | 0.91 | 0.88 | [61] |
| 640 | Nc1ccccc1 | CCOC(=O)C | -1.14 | -0.07 | -0.27 | -0.01 | 0.10 | 0.12 | -0.02 | 0.09 | 0.36 | [61] |
| 641 | Nc1ccccc1 | C1COCCO1 | -1.35 | -0.09 | -0.78 | -1.43 | -1.05 | -0.11 | -0.20 | -0.27 | -0.97 | [61] |

Continued on next page

**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 642 | Nc1ccccc1 | CC(C)=O | -1.35 | -0.26 | -0.40 | -0.42 | -0.22 | 0.19 | -0.20 | -0.21 | -0.22 | [61] |
| 643 | Nc1ccccc1 | CCC(C)=O | -1.24 | -0.14 | -0.30 | -0.29 | -0.29 | 0.28 | -0.04 | -0.09 | -0.49 | [61] |
| 644 | Nc1ccccc1 | CCCCl | 0.48 | 0.78 | 0.67 | 0.90 | 1.16 | | | | 1.07 | [61] |
| 645 | Nc1ccccc1 | CC(C)(C)Cl | 0.61 | 1.49 | 1.32 | 1.75 | 1.73 | | | | 1.55 | [61] |
| 646 | Nc1ccccc1 | ClCCl | -0.08 | -0.99 | -1.05 | -1.14 | 0.28 | -0.20 | -0.26 | 0.14 | 0.34 | [61] |
| 647 | Nc1ccccc1 | ClC(Cl)Cl | 0.13 | -1.66 | -1.71 | -2.81 | 0.38 | -0.06 | | 0.38 | 0.40 | [61] |
| 648 | Nc1ccccc1 | ClC(Cl)(Cl)Cl | 1.02 | 1.36 | 1.25 | 1.38 | 1.65 | 0.58 | 0.22 | 1.53 | 1.54 | [61] |
| 649 | Nc1ccccc1 | CCBr | 0.06 | -0.24 | -0.31 | 0.16 | 1.07 | 0.23 | | | 0.75 | [61] |
| 650 | Nc1ccccc1 | CCI | 0.08 | -0.13 | -0.16 | 0.07 | 1.55 | | | | 1.02 | [61] |
| 651 | Nc1ccccc1 | C(=S)=S | 0.58 | -0.87 | -0.82 | -1.02 | | 0.13 | -0.30 | | 1.24 | [61] |
| 652 | COc1ccccc1 | CCCCC | 0.98 | 1.21 | 1.11 | 0.95 | | 0.55 | 0.90 | 1.28 | 1.17 | [54 , 61 , 61] |
| 653 | COc1ccccc1 | CCCCCC | 1.11 | 1.39 | 1.28 | 1.03 | | 0.60 | 0.76 | 1.35 | 1.33 | [54 , 61] |
| 654 | COc1ccccc1 | C1CCCCC1 | 0.88 | 1.09 | 1.08 | 0.92 | | 0.22 | 0.11 | 1.00 | 1.01 | [54 , 61 , 61] |
| 655 | COc1ccccc1 | CCCC(C)C | 1.07 | 1.39 | 1.28 | 1.03 | | | | 1.46 | 1.32 | [54 , 61 , 61] |
| 656 | COc1ccccc1 | CCCCCCC | 1.22 | 1.54 | 1.46 | 1.10 | | 0.64 | 0.63 | 1.44 | 1.39 | [54 , 61 , 61] |
| 657 | COc1ccccc1 | CC(C)CC(C)C | 1.14 | 1.54 | 1.45 | 1.10 | | | | 1.66 | 1.45 | [54 , 61 , 61] |
| 658 | COc1ccccc1 | CCCCCCCC | 1.33 | 1.68 | 1.62 | 1.17 | | 0.70 | 0.58 | 1.53 | 1.49 | [54 , 61 , 61] |
| 659 | COc1ccccc1 | CC(C)C(C)C(C)C | 1.17 | 1.68 | 1.62 | 1.17 | | | | | 1.42 | [54 , 61 , 61] |
| 660 | COc1ccccc1 | CC(C)CCC(C)C | 1.28 | 1.68 | 1.62 | 1.17 | | | | | 1.56 | [54] |
| 661 | COc1ccccc1 | CCC1CCCCC1 | 1.09 | 1.42 | 1.42 | 1.05 | | | | 1.32 | 1.21 | [54 , 61 , 61] |
| 662 | COc1ccccc1 | CCCCCCCCC | 1.43 | 1.81 | 1.78 | 1.24 | | 0.76 | 0.52 | 1.61 | 1.59 | [54 , 61 , 61] |
| 663 | COc1ccccc1 | CCC(C)CCC(C)C | 1.35 | 1.80 | 1.77 | 1.24 | | | | | 1.46 | [61] |
| 664 | COc1ccccc1 | c1ccccc1 | -0.04 | 0.04 | 0.06 | -0.04 | | -0.03 | -0.21 | 0.01 | 0.05 | [61] |
| 665 | COc1ccccc1 | CCCC=C | 0.52 | 0.91 | 0.82 | 0.54 | | 0.31 | 0.90 | 0.93 | 0.87 | [61] |
| 666 | COc1ccccc1 | CC(C)C=C | 0.55 | 0.91 | 0.82 | 0.54 | | | | | 0.80 | [61] |
| 667 | COc1ccccc1 | CC(=C)C=C | 0.17 | 0.70 | 0.64 | 0.29 | | | | | 0.43 | [61] |
| 668 | COc1ccccc1 | CO | 2.57 | 1.36 | 1.35 | 1.49 | | 0.25 | 3.96 | 3.06 | 2.36 | [61] |
| 669 | COc1ccccc1 | CCO | 2.54 | 1.56 | 1.19 | 1.49 | | 0.30 | 1.80 | 2.51 | 2.26 | [61] |
| 670 | COc1ccccc1 | CCOC(=O)C | 0.02 | -0.13 | -0.29 | -0.15 | | -0.13 | -0.26 | 0.13 | 0.08 | [61] |
| 671 | COc1ccccc1 | CCCCl | 0.10 | 0.67 | 0.60 | 0.06 | | | | | 0.13 | [61] |
| 672 | COc1ccccc1 | ClCCl | -0.25 | -0.92 | -0.92 | -0.87 | | -0.34 | -0.34 | -0.40 | -0.26 | [61] |
| 673 | COc1ccccc1 | ClC(Cl)Cl | -0.15 | -0.87 | -0.87 | -3.51 | | -0.27 | | -0.62 | -0.39 | [61] |
| 674 | COc1ccccc1 | ClC(Cl)(Cl)Cl | 0.74 | 0.36 | 0.29 | -0.21 | | 0.10 | -0.11 | 0.28 | 0.25 | [61] |
| 675 | COc1ccccc1 | CCBr | -0.31 | -0.19 | -0.22 | 0.08 | | -0.11 | | | 0.08 | [61] |
| 676 | COc1ccccc1 | CCI | -0.36 | 0.06 | 0.06 | -0.02 | | | | | 0.11 | [61] |
| 677 | COc1ccccc1 | C(=S)=S | 0.18 | 0.41 | 0.51 | 0.41 | | -0.08 | -0.34 | | 0.48 | [61] |
| 678 | c1ccccc1 | CCCCC | 0.64 | 0.63 | 0.48 | 0.77 | 0.69 | 0.31 | 0.44 | 0.84 | 0.71 | [54 , 61 , 61 , 78] |
| 679 | c1ccccc1 | C1CCCC1 | 0.48 | 0.43 | 0.40 | 0.51 | 0.37 | -0.08 | -0.03 | 0.49 | 0.44 | [78] |
| 680 | c1ccccc1 | CCCCCC | 0.68 | 0.66 | 0.54 | 0.77 | 0.71 | 0.31 | 0.35 | 0.81 | 0.78 | [54 , 61 , 61 , 106 , 106 , 107] |
| 681 | c1ccccc1 | C1CCCCC1 | 0.52 | 0.48 | 0.46 | 0.55 | 0.45 | -0.06 | -0.04 | 0.57 | 0.57 | [54 , 61 , 61 , 78 , 108] |
| 682 | c1ccccc1 | CCCC(C)C | 0.66 | 0.66 | 0.54 | 0.77 | 0.77 | | | 0.92 | 0.80 | [54 , 61 , 61] |
| 683 | c1ccccc1 | CC1CCCC1 | 0.55 | 0.48 | 0.46 | 0.52 | 0.38 | | | 0.60 | 0.50 | [78 , 108] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 684 | c1ccccc1 | CCCCCCC | 0.72 | 0.67 | 0.59 | 0.76 | 0.74 | 0.28 | 0.27 | 0.80 | 0.76 | [54 , 61 , 61 , 78 , 109 , 110] |
| 685 | c1ccccc1 | CC(C)CC(C)C | 0.68 | 0.66 | 0.59 | 0.76 | 0.82 | | | 1.02 | 0.87 | [54 , 61 , 61] |
| 686 | c1ccccc1 | CC1CCCCC1 | 0.57 | 0.51 | 0.52 | 0.57 | 0.39 | 0.07 | 0.10 | 0.65 | 0.59 | [78] |
| 687 | c1ccccc1 | CCCCCCCC | 0.75 | 0.66 | 0.64 | 0.75 | 0.80 | 0.29 | 0.24 | 0.79 | 0.78 | [54 , 61 , 61 , 61 , 78 , 110] |
| 688 | c1ccccc1 | C1CCCCCCC1 | 0.50 | 0.51 | 0.57 | 0.61 | 0.18 | -0.06 | -0.08 | 0.67 | 0.62 | [65] |
| 689 | c1ccccc1 | CC(C)C(C)C(C)C | 0.65 | 0.65 | 0.64 | 0.75 | 0.54 | | | | 0.82 | [54 , 61] |
| 690 | c1ccccc1 | CC(C)CCC(C)C | 0.73 | 0.65 | 0.64 | 0.75 | | | | | 0.78 | [54] |
| 691 | c1ccccc1 | CCC1CCCCC1 | 0.59 | 0.51 | 0.57 | 0.57 | | | | 0.67 | 0.67 | [54 , 61 , 61] |
| 692 | c1ccccc1 | CCCCCCCCC | 0.77 | 0.64 | 0.68 | 0.74 | 0.95 | 0.29 | 0.22 | 0.78 | 0.85 | [54 , 61 , 61] |
| 693 | c1ccccc1 | CCCCCCCCCCCCCC | 0.85 | 0.41 | 0.84 | 0.70 | 0.90 | 0.33 | 0.15 | 0.67 | 0.60 | [111] |
| 694 | c1ccccc1 | Cc1ccccc1 | -0.04 | -0.05 | -0.04 | 0.01 | -0.05 | -0.14 | -0.15 | 0.04 | -0.08 | [61] |
| 695 | c1ccccc1 | Cc1ccc(C)cc1 | -0.08 | -0.16 | -0.12 | 0.03 | -0.08 | -0.09 | -0.12 | 0.07 | 0.06 | [112] |
| 696 | c1ccccc1 | CCCC=C | 0.28 | 0.46 | 0.33 | 0.49 | 0.58 | 0.43 | 0.44 | 0.60 | 0.53 | [111] |
| 697 | c1ccccc1 | CC(C)C=C | 0.31 | 0.46 | 0.33 | 0.49 | | | | | 0.51 | [61] |
| 698 | c1ccccc1 | CC(=C)C=C | 0.10 | 0.41 | 0.29 | 0.29 | 0.39 | | | | 0.22 | [61] |
| 699 | c1ccccc1 | CO | 3.63 | 2.81 | 2.68 | 3.05 | 3.38 | 1.01 | 3.94 | 3.90 | 2.97 | [113] |
| 700 | c1ccccc1 | CCO | 3.43 | 2.38 | 1.90 | 3.00 | 3.01 | 1.12 | 1.98 | 3.34 | 2.78 | [61 , 113 , 113] |
| 701 | c1ccccc1 | CCOC(=O)C | 0.22 | 0.14 | -0.07 | 0.17 | 0.42 | 0.34 | -0.22 | 0.43 | 0.23 | [61] |
| 702 | c1ccccc1 | CCCCOC(=O)C | 0.04 | -0.07 | -0.22 | -0.08 | 0.10 | 0.36 | -0.07 | -0.03 | 0.04 | [61] |
| 703 | c1ccccc1 | C1COCCO1 | 0.13 | 0.82 | 0.10 | -0.27 | -0.24 | -0.03 | -0.06 | -0.02 | -0.03 | [61] |
| 704 | c1ccccc1 | CC(C)=O | 0.72 | 0.43 | 0.25 | 0.36 | 0.78 | 0.49 | -0.17 | 0.42 | 0.52 | [61] |
| 705 | c1ccccc1 | CCC(C)=O | 0.49 | 0.29 | 0.10 | 0.22 | 0.36 | 0.43 | -0.19 | 0.16 | 0.20 | [61] |
| 706 | c1ccccc1 | CCCCl | 0.20 | 0.02 | -0.12 | 0.12 | 0.15 | | | | 0.06 | [61] |
| 707 | c1ccccc1 | CC(C)(C)Cl | 0.29 | 0.30 | 0.11 | 0.33 | 0.31 | | | | 0.23 | [61] |
| 708 | c1ccccc1 | ClCCl | 0.18 | -0.24 | -0.33 | -0.04 | -0.03 | -0.07 | -0.19 | -0.13 | -0.08 | [61] |
| 709 | c1ccccc1 | ClC(Cl)Cl | 0.20 | -0.31 | -0.39 | -0.19 | -0.13 | -0.11 | | -0.36 | -0.21 | [61] |
| 710 | c1ccccc1 | ClC(Cl)(Cl)Cl | 0.57 | 0.10 | -0.02 | 0.13 | 0.06 | -0.15 | -0.15 | 0.10 | 0.12 | [61] |
| 711 | c1ccccc1 | CCBr | -0.20 | -0.05 | -0.16 | 0.22 | 0.13 | 0.14 | | | 0.01 | [61] |
| 712 | c1ccccc1 | CCC#N | 1.21 | 0.55 | 0.41 | 0.54 | 1.07 | 0.81 | 0.10 | 0.75 | 0.64 | [61 , 101] |
| 713 | c1ccccc1 | CCCC#N | 0.85 | 0.39 | 0.25 | 0.40 | | 0.88 | -0.07 | 0.41 | 0.29 | [101] |
| 714 | c1ccccc1 | C[N+]([O-])=O | 1.68 | 1.22 | 1.08 | 1.16 | 1.72 | 0.92 | 1.20 | 1.37 | 1.25 | [61] |
| 715 | c1ccccc1 | CCI | -0.30 | 0.10 | 0.04 | 0.08 | 0.48 | | | | 0.11 | [61] |
| 716 | c1ccccc1 | CCN(CC)CC | 0.32 | -0.13 | -0.21 | 0.37 | 0.21 | -0.08 | -0.08 | 0.36 | 0.26 | [61] |
| 717 | c1ccccc1 | C(=S)=S | -0.06 | 0.34 | 0.36 | 0.43 | | -0.24 | -0.16 | | 0.39 | [61] |
| 718 | c1ccccc1 | C[S](C)=O | 2.20 | 1.51 | 1.38 | 1.52 | | 1.19 | 2.14 | 1.35 | 4.65 | [114] |
| 719 | N#Cc1ccccc1 | CCCCC | 1.87 | | | | 1.65 | 0.71 | 0.14 | 1.72 | 1.62 | [54 , 61 , 61] |
| 720 | N#Cc1ccccc1 | CCCCCC | 2.13 | | | | 1.85 | 0.78 | 0.08 | 1.90 | 1.80 | [54 , 61 , 61 , 47] |
| 721 | N#Cc1ccccc1 | C1CCCCC1 | 1.73 | | | | 1.53 | 0.42 | -0.17 | 1.64 | 1.54 | [54 , 61 , 61 , 47] |
| 722 | N#Cc1ccccc1 | CCCC(C)C | 2.06 | | | | 1.85 | | | 1.96 | 1.84 | [54 , 61 , 61] |
| 723 | N#Cc1ccccc1 | CCCCCCC | 2.37 | | | | 2.03 | 0.85 | 0.03 | 2.09 | 1.94 | [54 , 61 , 61] |
| 724 | N#Cc1ccccc1 | CC(C)CC(C)C | 2.24 | | | | 1.99 | | | 2.19 | 2.03 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 725 | N#Cc1ccccc1 | CCCCCCCC | 2.60 | | | | 2.26 | 0.94 | 0.02 | 2.27 | 2.08 | [54 , 61 , 61 , 61] |
| 726 | N#Cc1ccccc1 | CC(C)C(C)C(C)C | 2.33 | | | | 1.93 | | | | 2.04 | [54 , 61 , 61] |
| 727 | N#Cc1ccccc1 | CC(C)CCC(C)C | 2.52 | | | | | | | | 2.22 | [54] |
| 728 | N#Cc1ccccc1 | CCC1CCCCC1 | 2.17 | | | | | | | 2.10 | 1.85 | [54 , 61 , 61] |
| 729 | N#Cc1ccccc1 | CCCCCCCCC | 2.83 | | | | 2.57 | 1.03 | 0.00 | 2.45 | 2.26 | [54 , 61 , 61] |
| 730 | N#Cc1ccccc1 | CCC(C)CCC(C)C | 2.69 | | | | | | | | 2.12 | [61] |
| 731 | N#Cc1ccccc1 | c1ccccc1 | 0.35 | | | | 0.30 | 0.23 | -0.16 | 0.22 | 0.22 | [47 , 115] |
| 732 | N#Cc1ccccc1 | Cc1ccccc1 | 0.55 | | | | 0.41 | 0.21 | -0.15 | 0.44 | 0.27 | [61 , 115] |
| 733 | N#Cc1ccccc1 | CCCC=C | 1.20 | | | | 1.36 | 0.52 | 0.13 | 1.24 | 1.26 | [61] |
| 734 | N#Cc1ccccc1 | CC=C(C)C | 1.18 | | | | | 0.38 | 0.02 | | 1.08 | [47] |
| 735 | N#Cc1ccccc1 | CC(C)C=C | 1.22 | | | | | | | | 1.11 | [61] |
| 736 | N#Cc1ccccc1 | CC(=C)C=C | 0.77 | | | | 0.93 | | | | 0.73 | [61 , 47] |
| 737 | N#Cc1ccccc1 | CO | 1.94 | | | | 1.54 | 0.42 | 5.85 | 2.05 | 1.53 | [61] |
| 738 | N#Cc1ccccc1 | CCO | 1.99 | | | | 1.58 | 0.57 | 3.24 | 1.65 | 1.52 | [61] |
| 739 | N#Cc1ccccc1 | C1COCCO1 | -0.01 | | | | -0.48 | 0.16 | 0.20 | 0.03 | -0.20 | [61] |
| 740 | N#Cc1ccccc1 | CCC(C)=O | 0.04 | | | | 0.03 | -0.17 | -0.08 | 0.00 | -0.13 | [61] |
| 741 | N#Cc1ccccc1 | ClCCl | -0.58 | | | | -0.45 | -0.27 | 0.03 | -0.62 | -0.36 | [61] |
| 742 | N#Cc1ccccc1 | CCBr | -0.48 | | | | 0.39 | -0.27 | | | 0.28 | [61] |
| 743 | N#Cc1ccccc1 | CCI | -0.56 | | | | 0.89 | | | | 0.45 | [61] |
| 744 | N#Cc1ccccc1 | C(=S)=S | -0.15 | | | | | 0.10 | 0.09 | | 0.83 | [61] |
| 745 | CC(=O)OCC1=CC=CC=C1 | CCCCCC | 1.31 | 1.07 | 1.01 | 1.15 | | 0.69 | 1.32 | 1.61 | 1.66 | [61 , 116] |
| 746 | CC(=O)OCC1=CC=CC=C1 | C1CCCCC1 | 1.05 | 0.81 | 0.83 | 0.97 | | 0.22 | 0.34 | 1.23 | 1.24 | [61 , 116] |
| 747 | CC(=O)OCC1=CC=CC=C1 | c1ccccc1 | 0.04 | -0.13 | -0.06 | -0.07 | | -0.08 | -0.20 | 0.00 | 0.04 | [61 , 116] |
| 748 | CC(=O)OCC1=CC=CC=C1 | C1C=CC=C1 | 0.04 | 0.17 | 0.25 | 0.30 | | | | | 0.78 | [61 , 116] |
| 749 | CC(=O)OCC1=CC=CC=C1 | CC(=C)C=C | 0.27 | 0.33 | 0.35 | 0.27 | | | | | 0.52 | [61 , 116] |
| 750 | CC(=O)OCC1=CC=CC=C1 | CCOC(=O)C | -0.03 | 0.00 | -0.07 | 0.08 | | -0.21 | -0.27 | -0.04 | 0.00 | [116 , 116] |
| 751 | CC(=O)OCC1=CC=CC=C1 | CC(C)=O | 0.10 | -0.05 | -0.04 | 0.07 | | -0.17 | -0.42 | -0.12 | 0.11 | [116 , 116] |
| 752 | CC(=O)OCC1=CC=CC=C1 | CCCCl | 0.06 | -0.06 | -0.05 | 0.08 | | | | | 0.20 | [116 , 116] |
| 753 | CC(=O)OCC1=CC=CC=C1 | CC(C)(C)Cl | 0.14 | 0.44 | 0.37 | 0.48 | | | | | 0.52 | [116 , 116] |
| 754 | CC(=O)OCC1=CC=CC=C1 | ClCCCl | -0.27 | -0.29 | -0.25 | -0.20 | | -0.34 | -0.36 | -0.43 | -0.34 | [116] |
| 755 | CC(=O)OCC1=CC=CC=C1 | ClC(Cl)Cl | -0.63 | -0.71 | -0.63 | -2.04 | | -0.34 | | -0.87 | -0.67 | [116 , 116] |
| 756 | CC(=O)OCC1=CC=CC=C1 | ClC(Cl)(Cl)Cl | 0.77 | 0.11 | 0.11 | 0.06 | | 0.06 | -0.01 | 0.36 | 0.34 | [116 , 116] |
| 757 | CC(=O)OCC1=CC=CC=C1 | CCBr | -0.43 | -0.22 | -0.17 | 0.14 | | -0.26 | | | 0.02 | [116 , 116] |
| 758 | CC(=O)OCC1=CC=CC=C1 | CC#N | 0.54 | 0.44 | 0.56 | 0.21 | | 0.02 | 0.49 | 0.18 | 0.41 | [116] |
| 759 | CC(=O)OCC1=CC=CC=C1 | CI | -0.51 | -0.07 | 0.13 | 0.20 | | | | 0.13 | 0.12 | [116] |
| 760 | CC(=O)OCC1=CC=CC=C1 | CCI | -0.43 | 0.09 | 0.16 | 0.09 | | | | | 0.28 | [116 , 116] |
| 761 | C1=CC=C(C=C1)CO | CCCCC | 1.72 | 1.49 | 1.48 | 2.12 | | 1.84 | 4.27 | 2.42 | 2.36 | [54 , 61 , 117] |
| 762 | C1=CC=C(C=C1)CO | C1CCCC1 | 1.41 | 1.17 | 1.19 | 1.83 | | 0.90 | 2.66 | 1.77 | 1.77 | [117] |
| 763 | C1=CC=C(C=C1)CO | CCCCCC | 1.95 | 1.74 | 1.73 | 2.30 | | 2.04 | 3.95 | 2.64 | 2.59 | [54 , 61 , 47 , 117] |
| 764 | C1=CC=C(C=C1)CO | C1CCCCC1 | 1.61 | 1.45 | 1.45 | 2.20 | | 1.34 | 2.49 | 2.07 | 2.06 | [54 , 61 , 47 , 117] |
| 765 | C1=CC=C(C=C1)CO | CCCC(C)C | 1.89 | 1.74 | 1.73 | 2.30 | | | | 2.76 | 2.58 | [54 , 61] |
| 766 | C1=CC=C(C=C1)CO | CC1CCCC1 | 1.65 | 1.44 | 1.44 | 1.89 | | | | 2.16 | 2.09 | [117] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 767 | C1=CC=C(C=C1)CO | CCCCCCC | 2.18 | 1.98 | 1.97 | 2.48 | | 2.24 | 3.65 | 2.87 | 2.81 | [54 , 61] |
| 768 | C1=CC=C(C=C1)CO | CC(C)CC(C)C | 2.05 | 1.97 | 1.96 | 2.48 | | | | 3.11 | 2.85 | [54 , 61] |
| 769 | C1=CC=C(C=C1)CO | CCCCCCCC | 2.40 | 2.19 | 2.20 | 2.65 | | 2.46 | 3.51 | 3.11 | 3.00 | [54 , 61 , 61] |
| 770 | C1=CC=C(C=C1)CO | CC(C)C(C)C(C)C | 2.13 | 2.19 | 2.19 | 2.65 | | | | | 2.86 | [54 , 61] |
| 771 | C1=CC=C(C=C1)CO | CC(C)CCC(C)C | 2.30 | 2.19 | 2.20 | 2.65 | | | | | 3.07 | [54] |
| 772 | C1=CC=C(C=C1)CO | CCC1CCCCC1 | 2.02 | 1.93 | 1.93 | 2.44 | | | | 2.72 | 2.56 | [54 , 61] |
| 773 | C1=CC=C(C=C1)CO | CCCCCCCCC | 2.61 | 2.40 | 2.43 | 2.83 | | 2.68 | 3.37 | 3.35 | 3.30 | [54 , 61] |
| 774 | C1=CC=C(C=C1)CO | CCC(C)CCC(C)C | 2.47 | 2.40 | 2.42 | 2.83 | | | | | 3.06 | [61] |
| 775 | C1=CC=C(C=C1)CO | c1ccccc1 | 0.66 | 0.57 | 0.55 | 0.73 | | 0.72 | 1.42 | 0.69 | 0.91 | [61 , 47 , 117] |
| 776 | C1=CC=C(C=C1)CO | Cc1ccccc1 | 0.86 | 0.74 | 0.70 | 0.89 | | 0.85 | 1.65 | 0.94 | 1.00 | [61] |
| 777 | C1=CC=C(C=C1)CO | CC=C(C)C | 1.20 | 1.37 | 1.33 | 1.73 | | 0.98 | 3.86 | | 1.83 | [61 , 47] |
| 778 | C1=CC=C(C=C1)CO | CC(=C)C=C | 0.88 | 1.03 | 1.06 | 0.99 | | | | | 1.46 | [61 , 47] |
| 779 | C1=CC=C(C=C1)CO | CCO | 0.17 | 0.23 | 0.07 | 0.27 | | -0.15 | -0.26 | -0.06 | 0.02 | [61] |
| 780 | C1=CC=C(C=C1)CO | C1COCCO1 | -0.56 | 0.63 | 0.27 | 0.66 | | 0.07 | 0.54 | -0.60 | -0.76 | [61] |
| 781 | C1=CC=C(C=C1)CO | CCC(C)=O | -0.48 | 0.17 | 0.17 | 0.27 | | 0.34 | 1.15 | -0.39 | -0.25 | [61] |
| 782 | C1=CC=C(C=C1)CCl | CCCCC | 0.92 | 0.96 | 0.81 | 1.12 | | 0.72 | 1.35 | | 1.39 | [61] |
| 783 | C1=CC=C(C=C1)CCl | CCCCCC | 1.05 | 1.10 | 0.95 | 1.21 | | 0.77 | 1.17 | | 1.46 | [61] |
| 784 | C1=CC=C(C=C1)CCl | CCCC=C | 0.43 | 0.59 | 0.47 | 0.80 | | 0.65 | 1.35 | | 5.55 | [61] |
| 785 | C1=CC=C(C=C1)CCl | CC(C)C=C | 0.45 | 0.59 | 0.47 | 0.80 | | | | | 0.81 | [61] |
| 786 | C1=CC=C(C=C1)CCl | CC(=C)C=C | 0.18 | 0.36 | 0.28 | 0.55 | | | | | 0.64 | [61] |
| 787 | C1=CC=C(C=C1)CCl | CO | 2.92 | 2.42 | 2.40 | 2.72 | | 0.55 | 3.45 | | 2.59 | [61] |
| 788 | C1=CC=C(C=C1)CCl | CCO | 2.78 | 2.28 | 1.86 | 2.54 | | 0.71 | 1.39 | | 2.45 | [61] |
| 789 | C1=CC=C(C=C1)CCl | CCCCl | 0.04 | 0.12 | 0.02 | 0.27 | | | | | 0.20 | [61] |
| 790 | C1=CC=C(C=C1)CCl | CC(C)(C)Cl | 0.06 | 0.57 | 0.39 | 0.60 | | | | | 0.39 | [61] |
| 791 | C1=CC=C(C=C1)CCl | ClCCl | -0.07 | -0.36 | -0.37 | -0.02 | | -0.33 | -0.39 | | -0.16 | [61] |
| 792 | C1=CC=C(C=C1)CCl | ClC(Cl)Cl | 0.10 | -0.67 | -0.69 | -0.29 | | -0.16 | | | -0.19 | [61] |
| 793 | C1=CC=C(C=C1)CCl | CCBr | -0.33 | -0.15 | -0.20 | 0.24 | | -0.22 | | | 0.03 | [61] |
| 794 | C1=CC=C(C=C1)CCl | C(=S)=S | 0.25 | 0.52 | 0.63 | 0.40 | | -0.17 | -0.42 | | 0.46 | [61] |
| 795 | C1=CC=C(C=C1)CC#N | CCCCC | 1.90 | 1.64 | 1.51 | 2.45 | | | | | 2.39 | [47] |
| 796 | C1=CC=C(C=C1)CC#N | CCC(C)C | 1.83 | 1.64 | 1.51 | 2.45 | | | | | 2.45 | [47] |
| 797 | C1=CC=C(C=C1)CC#N | CCCCCC | 2.17 | 1.91 | 1.77 | 2.66 | | | | | 2.55 | [47] |
| 798 | C1=CC=C(C=C1)CC#N | C1CCCCC1 | 1.77 | 1.50 | 1.48 | 2.31 | | | | | 2.07 | [47] |
| 799 | C1=CC=C(C=C1)CC#N | c1ccccc1 | 0.38 | 0.19 | 0.22 | 0.41 | | | | | 0.47 | [47] |
| 800 | C1=CC=C(C=C1)CC#N | CC=C(C)C | 1.18 | 1.44 | 1.24 | 1.89 | | | | | 1.66 | [47] |
| 801 | C1=CC=C(C=C1)CC#N | CC(=C)C=C | 0.75 | 0.81 | 0.74 | 0.81 | | | | | 1.12 | [47] |
| 802 | CC(=O)CCc1ccccc1 | CCCCC | 1.17 | 0.78 | 0.73 | 1.47 | | | | | 1.65 | [47] |
| 803 | CC(=O)CCc1ccccc1 | CCC(C)C | 1.12 | 0.77 | 0.73 | 1.47 | | | | | 1.65 | [47] |
| 804 | CC(=O)CCc1ccccc1 | CCCCCC | 1.36 | 0.95 | 0.88 | 1.61 | | | | | 1.79 | [47] |
| 805 | CC(=O)CCc1ccccc1 | C1CCCCC1 | 1.09 | 0.69 | 0.72 | 1.48 | | | | | 1.37 | [47] |
| 806 | CC(=O)CCc1ccccc1 | c1ccccc1 | -0.03 | -0.12 | -0.03 | -0.02 | | | | | 0.03 | [47] |
| 807 | CC(=O)CCc1ccccc1 | CC=C(C)C | 0.64 | 0.63 | 0.52 | 1.05 | | | | | 1.06 | [47] |
| 808 | CC(=O)CCc1ccccc1 | CC(=C)C=C | 0.25 | 0.21 | 0.22 | 0.37 | | | | | 0.60 | [47] |
| 809 | NCc1ccccc1 | CCCCCC | 1.63 | 1.35 | 1.23 | 1.88 | | 1.68 | 2.70 | | 2.09 | [47] |
| 810 | NCc1ccccc1 | C1CCCCC1 | 1.33 | 1.04 | 1.03 | 1.45 | | 0.96 | 1.47 | | 1.62 | [47] |
| 811 | NCc1ccccc1 | c1ccccc1 | 0.22 | 0.09 | 0.11 | 0.25 | | 0.39 | 0.62 | | 0.36 | [47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 812 | NCc1ccccc1 | CC=C(C)C | 0.90 | 1.08 | 0.90 | 1.35 | | 0.85 | 2.61 | | 1.39 | [47] |
| 813 | NCc1ccccc1 | CC(=C)C=C | 0.49 | 0.71 | 0.65 | 0.55 | | | | | 0.93 | [47] |
| 814 | C1CCC(CC1)C2CCCCC2 | CCCCCC | 0.01 | 0.00 | -0.05 | 0.15 | | 0.13 | 0.74 | 0.17 | 0.18 | [118] |
| 815 | C1CCC(CC1)C2CCCCC2 | C1CCCCC1 | -0.05 | -0.15 | -0.08 | -0.03 | | -0.29 | -0.13 | -0.15 | 0.01 | [118] |
| 816 | C1CCC(CC1)C2CCCCC2 | CCCCCCC | 0.02 | 0.05 | -0.03 | 0.16 | | 0.12 | 0.56 | 0.17 | 0.12 | [118] |
| 817 | C1CCC(CC1)C2CCCCC2 | c1ccccc1 | 0.33 | 0.11 | 0.26 | 0.25 | | -0.43 | -0.46 | 0.25 | 0.26 | [118] |
| 818 | C1CCC(CC1)C2CCCCC2 | CCCCC=C | 0.03 | 0.03 | 0.00 | 0.22 | | 0.16 | 0.81 | 0.09 | 0.14 | [118] |
| 819 | C1CCC(CC1)C2CCCCC2 | C1CCC=CC1 | -0.04 | -0.14 | -0.04 | -0.03 | | -0.19 | -0.37 | | -0.04 | [118] |
| 820 | C1CCC(CC1)C2CCCCC2 | C1CC=CC=C1 | 0.09 | -0.24 | 0.02 | 0.21 | | | | | 0.07 | [118] |
| 821 | C1CCC(CC1)C2CCCCC2 | C1C=CCC=C1 | 0.10 | -0.24 | 0.02 | 0.21 | | | | | -0.01 | [118] |
| 822 | C1CCC(CC1)C2CCCCC2 | CCCCCC=C | 0.04 | 0.08 | 0.02 | 0.24 | | 0.23 | 0.57 | | 0.16 | [118] |
| 823 | C1CCC(CC1)C2CCCCC2 | CCCCC#C | 0.41 | 1.31 | 1.24 | -0.49 | | | | | 0.44 | [118] |
| 824 | C1CCC(CC1)C2CCCCC2 | CCCCCC#C | 0.37 | 1.26 | 1.16 | -0.53 | | | | | 0.46 | [118] |
| 825 | COc1ccccc1Br | CCCCCC | | 1.89 | 1.75 | 1.17 | | 1.48 | 2.82 | | 1.45 | [116] |
| 826 | COc1ccccc1Br | C1CCCCC1 | | 1.48 | 1.47 | 1.27 | | 0.73 | 1.46 | | 1.11 | [116] |
| 827 | COc1ccccc1Br | c1ccccc1 | | -0.04 | 0.00 | -0.09 | | 0.24 | 0.54 | | 0.13 | [116] |
| 828 | COc1ccccc1Br | C1C=CC=C1 | | 0.84 | 0.90 | 0.62 | | | | | 0.90 | [116] |
| 829 | COc1ccccc1Br | CC(=C)C=C | | 1.13 | 1.08 | 0.58 | | | | | 0.58 | [116] |
| 830 | COc1ccccc1Br | CCOC(=O)C | | -0.14 | -0.31 | -0.04 | | 0.03 | 0.41 | | 0.17 | [116] |
| 831 | COc1ccccc1Br | CC(C)=O | | 0.01 | -0.07 | -0.16 | | -0.03 | -0.03 | | 0.33 | [116] |
| 832 | COc1ccccc1Br | CCCCl | | 0.59 | 0.52 | 0.15 | | | | | 0.34 | [116] |
| 833 | COc1ccccc1Br | CC(C)(C)Cl | | 1.19 | 1.04 | 0.52 | | | | | 0.61 | [116] |
| 834 | COc1ccccc1Br | ClCCCl | | 0.39 | 0.36 | -0.08 | | -0.30 | -0.19 | | 0.12 | [116] |
| 835 | COc1ccccc1Br | ClC(Cl)Cl | | -0.80 | -0.80 | -2.30 | | -0.12 | | | -0.84 | [116] |
| 836 | COc1ccccc1Br | ClC(Cl)(Cl)Cl | | 0.77 | 0.71 | -0.30 | | 0.45 | 0.88 | | 0.41 | [116] |
| 837 | COc1ccccc1Br | CCBr | | 0.05 | 0.03 | 0.17 | | -0.09 | | | 0.18 | [116] |
| 838 | COc1ccccc1Br | CC#N | | 0.29 | 0.31 | -0.01 | | 0.02 | -0.34 | | 1.01 | [116] |
| 839 | COc1ccccc1Br | CI | | -0.15 | 0.01 | -0.05 | | | | | 0.21 | [116] |
| 840 | COc1ccccc1Br | CCI | | 0.17 | 0.18 | -0.09 | | | | | 0.25 | [116] |
| 841 | Brc1ccccc1 | CCCCC | 1.21 | 1.36 | 1.18 | 1.03 | 1.00 | 1.16 | 1.26 | 0.95 | 0.87 | [61] |
| 842 | Brc1ccccc1 | CCCCCC | 1.37 | 1.55 | 1.36 | 1.08 | 1.05 | 1.22 | 1.09 | 0.94 | 0.89 | [61] |
| 843 | Brc1ccccc1 | C1CCCCC1 | 1.07 | 1.19 | 1.15 | 1.14 | 0.76 | 0.47 | 0.34 | 0.57 | 0.62 | [61] |
| 844 | Brc1ccccc1 | CCCC(C)C | 1.34 | 1.54 | 1.36 | 1.08 | 1.10 | | | 1.08 | 0.98 | [61] |
| 845 | Brc1ccccc1 | CCCCCCC | 1.52 | 1.71 | 1.54 | 1.12 | 1.10 | 1.25 | 0.94 | 0.95 | 0.92 | [61] |
| 846 | Brc1ccccc1 | CC(C)CC(C)C | 1.44 | 1.70 | 1.54 | 1.12 | 1.16 | | | 1.22 | 1.07 | [61] |
| 847 | Brc1ccccc1 | CCCCCCCC | 1.66 | 1.85 | 1.71 | 1.17 | 1.18 | 1.34 | 0.87 | 0.97 | 0.98 | [61] |
| 848 | Brc1ccccc1 | CC(C)C(C)C(C)C | 1.46 | 1.84 | 1.71 | 1.17 | 0.91 | | | | 0.99 | [61] |
| 849 | Brc1ccccc1 | CCC1CCCCC1 | 1.34 | 1.53 | 1.51 | 1.19 | | | | 0.76 | 0.76 | [61] |
| 850 | Brc1ccccc1 | CCCCCCCCC | 1.80 | 1.99 | 1.88 | 1.21 | 1.35 | 1.41 | 0.81 | 0.98 | 1.08 | [61] |
| 851 | Brc1ccccc1 | CCC(C)CCC(C)C | 1.71 | 1.98 | 1.88 | 1.21 | | | | | 1.02 | [61] |
| 852 | Brc1cccc2ccccc12 | CCCCCC | 1.42 | 1.56 | 1.17 | 1.37 | | 0.92 | 2.39 | | 1.59 | [116 , 61] |
| 853 | Brc1cccc2ccccc12 | C1CCCCC1 | 1.06 | 1.10 | 0.96 | 1.28 | | 0.22 | 1.09 | | 1.03 | [116 , 61] |
| 854 | Brc1cccc2ccccc12 | c1ccccc1 | 0.04 | -0.07 | -0.04 | -0.04 | | -0.17 | 0.24 | | 0.33 | [116 , 61] |
| 855 | Brc1cccc2ccccc12 | C1C=CC=C1 | 0.18 | 0.50 | 0.52 | 0.50 | | | | | 0.94 | [116 , 61] |
| 856 | Brc1cccc2ccccc12 | CC(=C)C=C | 0.46 | 0.86 | 0.64 | 0.60 | | | | | 0.72 | [116 , 116] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 857 | Brc1cccc2ccccc12 | CCOC(=O)C | 0.41 | 0.30 | -0.12 | 0.36 | | 0.22 | 0.13 | | 0.60 | [116 , 116] |
| 858 | Brc1cccc2ccccc12 | CC(C)=O | 0.72 | 0.34 | 0.08 | 0.07 | | 0.28 | -0.24 | | 0.76 | [116 , 116] |
| 859 | Brc1cccc2ccccc12 | CCCCl | 0.52 | 0.19 | -0.05 | 0.36 | | | | | 0.40 | [116 , 116] |
| 860 | Brc1cccc2ccccc12 | CC(C)(C)Cl | 0.70 | 0.84 | 0.44 | 0.70 | | | | | 0.76 | [116 , 116] |
| 861 | Brc1cccc2ccccc12 | ClCCCl | 0.65 | -0.16 | -0.34 | 0.10 | | -0.26 | -0.33 | | 0.36 | [116] |
| 862 | Brc1cccc2ccccc12 | ClC(Cl)Cl | 0.31 | -0.37 | -0.48 | -0.34 | | -0.24 | | | 0.12 | [116 , 116] |
| 863 | Brc1cccc2ccccc12 | ClC(Cl)(Cl)Cl | 0.58 | 0.53 | 0.28 | -0.02 | | -0.03 | 0.55 | | 0.45 | [116 , 116] |
| 864 | Brc1cccc2ccccc12 | CCBr | -0.07 | -0.01 | -0.16 | 0.36 | | -0.01 | | | 0.21 | [116 , 116] |
| 865 | Brc1cccc2ccccc12 | CC#N | 1.46 | 0.61 | 0.51 | 0.34 | | 0.46 | -0.16 | | 1.48 | [116] |
| 866 | Brc1cccc2ccccc12 | CI | -0.27 | -0.24 | -0.08 | -0.15 | | | | | 0.22 | [116] |
| 867 | Brc1cccc2ccccc12 | CCI | -0.20 | 0.08 | -0.02 | -0.06 | | | | | 0.20 | [116 , 116] |
| 868 | CCCCOC(=O)C | CCCCC | 0.66 | 0.59 | 0.61 | 0.67 | 0.53 | 0.19 | 0.22 | 0.68 | 0.65 | [54 , 61] |
| 869 | CCCCOC(=O)C | CCCCCC | 0.77 | 0.72 | 0.72 | 0.76 | 0.63 | 0.25 | 0.14 | 0.77 | 0.75 | [54 , 61 , 119] |
| 870 | CCCCOC(=O)C | C1CCCCC1 | 0.64 | 0.65 | 0.60 | 0.74 | 0.45 | 0.11 | -0.22 | 0.69 | 0.67 | [54 , 61] |
| 871 | CCCCOC(=O)C | CCCC(C)C | 0.73 | 0.72 | 0.72 | 0.76 | 0.66 | | | 0.81 | 0.76 | [54 , 61] |
| 872 | CCCCOC(=O)C | CCCCCCC | 0.86 | 0.82 | 0.82 | 0.85 | 0.73 | 0.31 | 0.07 | 0.87 | 0.89 | [54 , 61] |
| 873 | CCCCOC(=O)C | CC(C)CC(C)C | 0.79 | 0.82 | 0.82 | 0.85 | 0.76 | | | 0.94 | 0.84 | [54 , 61] |
| 874 | CCCCOC(=O)C | CCCCCCCC | 0.95 | 0.91 | 0.91 | 0.94 | 0.88 | 0.39 | 0.05 | 0.96 | 1.02 | [54 , 61] |
| 875 | CCCCOC(=O)C | CC(C)C(C)C(C)C | 0.82 | 0.91 | 0.91 | 0.94 | 0.58 | | | | 0.86 | [54 , 61] |
| 876 | CCCCOC(=O)C | CC(C)CCC(C)C | 0.89 | 0.91 | 0.91 | 0.94 | | | | | 0.92 | [54] |
| 877 | CCCCOC(=O)C | CCC1CCCCC1 | 0.81 | 0.88 | 0.80 | 0.90 | | | | 0.93 | 0.88 | [54 , 61] |
| 878 | CCCCOC(=O)C | CCCCCCCCC | 1.03 | 0.99 | 1.00 | 1.03 | 1.10 | 0.45 | 0.03 | 1.04 | 1.13 | [54] |
| 879 | CCCCOC(=O)C | c1ccccc1 | -0.06 | -0.08 | -0.17 | -0.15 | -0.04 | 0.01 | -0.25 | -0.13 | 0.76 | [120] |
| 880 | CCCCOC(=O)C | Cc1ccccc1 | 0.04 | 0.04 | -0.09 | 0.00 | -0.03 | 0.02 | -0.22 | -0.05 | -0.80 | [120] |
| 881 | CCCCOC(=O)C | Cc1cccc(C)c1 | 0.08 | 0.10 | -0.07 | 0.15 | 0.10 | 0.04 | -0.19 | | -0.48 | [120] |
| 882 | CCCCOC(=O)C | Cc1ccc(C)cc1 | 0.08 | 0.10 | -0.07 | 0.15 | 0.03 | 0.01 | -0.20 | 0.03 | -0.54 | [120] |
| 883 | CCCCOC(=O)C | Cc1ccccc1C | 0.06 | 0.10 | -0.07 | 0.15 | 0.04 | 0.03 | -0.19 | | -0.36 | [120] |
| 884 | CCCCOC(=O)C | CCCCCC=C | 0.44 | 0.50 | 0.49 | 0.51 | 0.54 | 0.02 | 0.07 | | 0.58 | [61] |
| 885 | CCCCOC(=O)C | ClC(Cl)(Cl)Cl | 0.42 | -0.04 | -0.01 | -0.01 | -0.04 | 0.09 | -0.27 | -0.11 | -0.06 | [61] |
| 886 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCC | | -0.06 | 0.15 | 0.37 | | | | | 0.19 | [121] |
| 887 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCC | | 0.10 | 0.28 | 0.48 | | | | | 0.28 | [121] |
| 888 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | C1CCCCC1 | | -0.09 | 0.16 | 0.36 | | | | | -0.11 | [121] |
| 889 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCC | | 0.26 | 0.39 | 0.58 | | | | | 0.35 | [121] |
| 890 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CC1CCCCC1 | | 0.08 | 0.29 | 0.41 | | | | | -0.02 | [121] |
| 891 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCCC | | 0.40 | 0.49 | 0.67 | | | | | 0.43 | [121] |
| 892 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCC1CCCCC1 | | 0.23 | 0.39 | 0.52 | | | | | 0.08 | [121] |
| 893 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | c1ccccc1 | | -0.73 | -0.42 | -0.56 | | | | | -0.45 | [121] |
| 894 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | Cc1ccccc1 | | -0.62 | -0.39 | -0.46 | | | | | -0.36 | [121] |
| 895 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCc1ccccc1 | | -0.46 | -0.26 | -0.31 | | | | | -0.30 | [121] |
| 896 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCC=C | | -0.33 | -0.08 | -0.01 | | | | | -0.05 | [121] |
| 897 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCC=C | | -0.15 | 0.04 | 0.10 | | | | | 0.03 | [121] |
| 898 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCC=C | | 0.00 | 0.15 | 0.22 | | | | | 0.10 | [121] |
| 899 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCC=C | | 0.13 | 0.25 | 0.32 | | | | | 0.18 | [121] |
| 900 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCC | 0.83 | 0.55 | 0.64 | 0.99 | | | | | 1.35 | [121] |
| 901 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCCC | 1.00 | 0.79 | 0.83 | 1.14 | | | | | 1.51 | [121] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 902 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | C1CCCCC1 | 0.74 | 0.46 | 0.64 | 0.91 | | | | | 1.01 | [121] |
| 903 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCCCC | 1.17 | 1.01 | 1.01 | 1.30 | | | | | 1.62 | [121] |
| 904 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CC1CCCCC1 | 0.89 | 0.69 | 0.82 | 1.00 | | | | | 1.12 | [121] |
| 905 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCCCCC | 1.32 | 1.21 | 1.18 | 1.44 | | | | | 1.81 | [121] |
| 906 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCC1CCCCC1 | 1.04 | 0.91 | 1.00 | 1.16 | | | | | 1.32 | [121] |
| 907 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | c1ccccc1 | -0.20 | -0.56 | -0.29 | -0.37 | | | | | -0.17 | [121] |
| 908 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | Cc1ccccc1 | -0.03 | -0.53 | -0.31 | -0.22 | | | | | -0.01 | [121] |
| 909 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCc1ccccc1 | 0.10 | -0.24 | -0.08 | 0.03 | | | | | 0.05 | [121] |
| 910 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCC=C | 0.35 | 0.20 | 0.31 | 0.47 | | | | | 0.83 | [121] |
| 911 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCC=C | 0.52 | 0.43 | 0.50 | 0.65 | | | | | 1.01 | [121] |
| 912 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCCC=C | 0.66 | 0.65 | 0.67 | 0.81 | | | | | 1.11 | [121] |
| 913 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2 | CCCCCCC=C | 0.85 | 0.85 | 0.84 | 0.97 | | | | | 1.34 | [121] |
| 914 | CCCC#N | CCCCC | 1.85 | 1.33 | 1.34 | 1.71 | | 1.16 | 1.09 | 1.71 | 1.62 | [54 , 61 , 61 , 98 , 74] |
| 915 | CCCC#N | CCCCCC | 2.12 | 1.51 | 1.54 | 1.83 | | 1.34 | 0.95 | 1.89 | 1.82 | [54 , 61 , 61 , 98] |
| 916 | CCCC#N | C1CCCCC1 | 1.81 | 1.35 | 1.30 | 1.64 | | 1.10 | 0.31 | 1.75 | 1.75 | [54 , 61 , 61 , 98] |
| 917 | CCCC#N | CCCC(C)C | 2.05 | 1.50 | 1.54 | 1.83 | | | | 1.92 | 4.86 | [54 , 61 , 61] |
| 918 | CCCC#N | CCCCCCC | 2.37 | 1.66 | 1.73 | 1.94 | | 1.52 | 0.82 | 2.07 | 1.99 | [54 , 61 , 61 , 98] |
| 919 | CCCC#N | CC(C)CC(C)C | 2.22 | 1.66 | 1.73 | 1.94 | | | | 2.12 | 1.94 | [54 , 61 , 61] |
| 920 | CCCC#N | CCCCCCCC | 2.62 | 1.80 | 1.91 | 2.06 | | 1.71 | 0.77 | 2.25 | 2.17 | [54 , 61 , 98] |
| 921 | CCCC#N | CC(C)C(C)C(C)C | 2.34 | 1.80 | 1.91 | 2.06 | | | | | 2.00 | [54 , 61 , 61] |
| 922 | CCCC#N | CC(C)CCC(C)C | 2.50 | 1.80 | 1.91 | 2.06 | | | | | 2.14 | [54] |
| 923 | CCCC#N | CCC1CCCCC1 | 2.26 | 1.67 | 1.69 | 1.81 | | | | 2.15 | 2.03 | [54 , 61] |
| 924 | CCCC#N | CCCCCCCCC | 2.86 | 1.92 | 2.09 | 2.17 | | 1.91 | 0.71 | 2.42 | 2.41 | [54 , 61] |
| 925 | CCCC#N | CCC(C)CCC(C)C | 2.71 | 1.92 | 2.09 | 2.17 | | | | | 2.06 | [61] |
| 926 | CCCC#N | Cc1ccccc1 | 0.71 | 0.52 | 0.38 | 0.47 | | 0.90 | 0.03 | 0.51 | 0.41 | [54] |
| 927 | CCCC#N | CCCC=C | 1.18 | 0.89 | 0.89 | 1.15 | | 0.73 | 1.09 | 1.24 | 1.19 | [74] |
| 928 | CCCC#N | CCO | 1.53 | 0.79 | 0.67 | 1.57 | | 0.46 | 1.00 | 1.29 | 1.25 | [61] |
| 929 | CCCC#N | C1COCCO1 | 0.04 | 0.21 | -0.01 | 0.35 | | 0.70 | -0.20 | 0.16 | 0.13 | [61] |
| 930 | CCCC#N | CCC(C)=O | -0.04 | -0.22 | -0.22 | -0.02 | | -0.11 | -0.12 | 0.08 | -0.06 | [61] |
| 931 | C(=S)=S | CCO | 4.66 | 2.85 | 2.56 | -1.39 | 4.22 | 1.63 | 0.68 | | 4.36 | [61 , 95] |
| 932 | C(=S)=S | C1COCCO1 | 1.20 | 1.61 | 1.21 | 0.95 | 1.04 | 0.18 | -0.12 | | 1.29 | [61] |
| 933 | C(=S)=S | CC(C)=O | 1.92 | 1.98 | 1.91 | 2.00 | 2.30 | 0.96 | -0.14 | | 2.12 | [61 , 95] |
| 934 | C(=S)=S | CCC(C)=O | 1.60 | 1.76 | 1.76 | 1.69 | 1.79 | 0.88 | -0.06 | | 1.48 | [61 , 95] |
| 935 | Clc1ccccc1 | CCCCC | 0.62 | 0.59 | 0.42 | 1.02 | 0.58 | 0.56 | 0.82 | 0.55 | 0.73 | [54 , 61 , 61] |
| 936 | Clc1ccccc1 | CCCCCC | 0.68 | 0.65 | 0.48 | 0.99 | 0.59 | 0.57 | 0.69 | 0.57 | 0.76 | [54 , 61 , 61] |
| 937 | Clc1ccccc1 | C1CCCCC1 | 0.49 | 0.44 | 0.41 | 1.00 | 0.40 | 0.09 | 0.10 | 0.53 | 0.57 | [54 , 61 , 61] |
| 938 | Clc1ccccc1 | CCCC(C)C | 0.66 | 0.65 | 0.48 | 0.99 | 0.65 | | | 0.62 | 2.35 | [54 , 61 , 61] |
| 939 | Clc1ccccc1 | CCCCCCC | 0.72 | 0.68 | 0.53 | 0.97 | 0.59 | 0.57 | 0.57 | 0.59 | 0.76 | [54 , 61 , 61] |
| 940 | Clc1ccccc1 | CC(C)CC(C)C | 0.69 | 0.67 | 0.53 | 0.97 | 0.69 | | | 0.67 | 0.88 | [54 , 61 , 61] |
| 941 | Clc1ccccc1 | CCCCCCCC | 0.77 | 0.70 | 0.58 | 0.94 | 0.64 | 0.60 | 0.52 | 0.60 | 0.80 | [54 , 61 , 61] |
| 942 | Clc1ccccc1 | CC(C)C(C)C(C)C | 0.68 | 0.69 | 0.58 | 0.94 | 0.39 | | | | 0.82 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 943 | Clc1ccccc1 | CC(C)CCC(C)C | 0.76 | 0.69 | 0.58 | 0.94 | | | | | 0.91 | [54] |
| 944 | Clc1ccccc1 | CCC1CCCCC1 | 0.59 | 0.52 | 0.51 | 0.94 | | | | 0.62 | 0.66 | [54 , 61 , 61] |
| 945 | Clc1ccccc1 | CCCCCCCCC | 0.80 | 0.70 | 0.62 | 0.92 | 0.77 | 0.63 | 0.48 | 0.62 | 0.80 | [54 , 61 , 61] |
| 946 | Clc1ccccc1 | CCC(C)CCC(C)C | 0.76 | 0.69 | 0.62 | 0.92 | | | | | 0.82 | [61] |
| 947 | Clc1ccccc1 | c1ccccc1 | -0.03 | 0.05 | 0.05 | 0.04 | -0.03 | -0.12 | -0.20 | 0.05 | 0.07 | [109 , 122] |
| 948 | ClC(Cl)Cl | CCCCC | 0.46 | 0.64 | 0.65 | 0.68 | 0.88 | 0.48 | 0.54 | 0.79 | 0.70 | [123 , 54 , 61 , 61 , 61 , 61] |
| 949 | ClC(Cl)Cl | CCCCCC | 0.47 | 0.67 | 0.73 | 0.69 | 0.96 | 0.50 | 0.44 | 0.80 | 0.65 | [54 , 61 , 61 , 61] |
| 950 | ClC(Cl)Cl | C1CCCCC1 | 0.34 | 0.61 | 0.63 | 0.45 | 0.86 | 0.16 | 0.03 | 0.75 | 0.48 | [54 , 61 , 61] |
| 951 | ClC(Cl)Cl | CCCC(C)C | 0.46 | 0.67 | 0.73 | 0.69 | 1.00 | | | 0.85 | 0.75 | [54] |
| 952 | ClC(Cl)Cl | CCCCCCC | 0.48 | 0.68 | 0.81 | 0.69 | 1.03 | 0.51 | 0.36 | 0.82 | 0.72 | [54] |
| 953 | ClC(Cl)Cl | CC(C)CC(C)C | 0.45 | 0.68 | 0.80 | 0.69 | 1.08 | | | 0.91 | 0.72 | [54 , 61 , 61] |
| 954 | ClC(Cl)Cl | CCCCCCCC | 0.47 | 0.68 | 0.87 | 0.69 | 1.15 | 0.55 | 0.32 | 0.83 | 0.70 | [54 , 61 , 61 , 61] |
| 955 | ClC(Cl)Cl | CC(C)C(C)C(C)C | 0.43 | 0.67 | 0.87 | 0.69 | 0.87 | | | | 0.69 | [54 , 61] |
| 956 | ClC(Cl)Cl | CC(C)CCC(C)C | 0.46 | 0.68 | 0.87 | 0.69 | | | | | 0.73 | [54] |
| 957 | ClC(Cl)Cl | CCC1CCCCC1 | 0.36 | 0.65 | 0.77 | 0.49 | | | | 0.83 | 0.59 | [54 , 61 , 61] |
| 958 | ClC(Cl)Cl | CCCCCCCCC | 0.46 | 0.66 | 0.93 | 0.69 | 1.34 | 0.58 | 0.29 | 0.84 | 0.73 | [54 , 61 , 61] |
| 959 | ClC(Cl)Cl | c1ccccc1 | 0.15 | -0.43 | -0.51 | -0.25 | 0.01 | -0.03 | -0.16 | -0.31 | -0.24 | [61 , 61 , 124] |
| 960 | ClC(Cl)Cl | Cc1ccccc1 | 0.07 | -0.42 | -0.46 | -0.27 | -0.01 | -0.02 | -0.11 | -0.37 | -0.39 | [61] |
| 961 | ClC(Cl)Cl | CO | 2.46 | 2.17 | 2.17 | 2.47 | 2.25 | 0.52 | 3.21 | 3.02 | 2.26 | [61 , 61 , 123] |
| 962 | ClC(Cl)Cl | CCO | 1.96 | 1.83 | 1.64 | 2.20 | 1.88 | 0.55 | 1.55 | 2.13 | 1.66 | [61] |
| 963 | ClC(Cl)Cl | C1COCCO1 | -1.20 | -1.77 | -2.04 | -2.81 | -1.83 | -0.13 | -0.11 | -1.77 | -1.51 | [61] |
| 964 | ClC(Cl)Cl | ClCCl | 0.13 | -0.02 | -0.01 | 0.05 | 0.00 | -0.21 | -0.21 | -0.06 | 0.23 | [61 , 61 , 123] |
| 965 | ClC(Cl)Cl | CC#N | -0.31 | 0.29 | 0.30 | 0.18 | 0.25 | 0.46 | 0.62 | 0.31 | 0.29 | [124] |
| 966 | ClC(Cl)Cl | CCN(CC)CC | -1.05 | -1.66 | -1.56 | -1.56 | -1.66 | 0.16 | -0.04 | -1.97 | -1.08 | [61] |
| 967 | Clc1cccc2ccccc12 | CCCCC | 0.76 | 0.72 | 0.36 | 1.49 | | 0.78 | 1.84 | | 1.35 | [47] |
| 968 | Clc1cccc2ccccc12 | CCC(C)C | 0.74 | 0.71 | 0.36 | 1.49 | | 1.07 | 2.42 | | 1.50 | [47] |
| 969 | Clc1cccc2ccccc12 | CCCCCC | 0.85 | 0.84 | 0.45 | 1.56 | | 0.82 | 1.61 | | 1.34 | [47] |
| 970 | Clc1cccc2ccccc12 | C1CCCCC1 | 0.59 | 0.50 | 0.36 | 1.37 | | 0.18 | 0.55 | | 0.67 | [47] |
| 971 | Clc1cccc2ccccc12 | c1ccccc1 | 0.00 | -0.06 | -0.03 | 0.10 | | -0.15 | -0.07 | | 0.39 | [47] |
| 972 | Clc1cccc2ccccc12 | CC=C(C)C | 0.36 | 0.75 | 0.30 | 1.08 | | 0.61 | 1.52 | | 0.93 | [47] |
| 973 | Clc1cccc2ccccc12 | CC(=C)C=C | 0.24 | 0.51 | 0.29 | 0.33 | | | | | 0.75 | [47] |
| 974 | O=C1CCC1 | CCCCCCC | 1.95 | 1.44 | 1.55 | 1.97 | | 1.64 | 1.33 | | 1.97 | [71] |
| 975 | C1CCCCCCCCC1 | CCCCCCC | 0.04 | 0.01 | -0.01 | 0.02 | | | | | 0.22 | [125] |
| 976 | C1CCCCCC1 | CCCCCCC | 0.02 | 0.03 | 0.00 | 0.07 | | | | 0.25 | 0.20 | [125] |
| 977 | C1CCCCCC1 | C1CCCC1 | -0.01 | -0.05 | -0.02 | -0.03 | | | | -0.04 | -0.01 | [126] |
| 978 | C1CCCCCC1 | C1CCCCC1 | 0.00 | -0.01 | -0.01 | -0.01 | | | | -0.01 | 0.01 | [126] |
| 979 | C1CCCCCC1 | CC(C)C(C)C | 0.03 | 0.04 | 0.00 | 0.08 | | | | 0.45 | 0.22 | [127] |
| 980 | OC1CCCCCC1 | CCCCC | 1.00 | 0.77 | 0.79 | 0.96 | | | | | 1.59 | [117] |
| 981 | OC1CCCCCC1 | C1CCCC1 | 0.82 | 0.59 | 0.62 | 0.71 | | | | | 1.08 | [117] |
| 982 | OC1CCCCCC1 | CCCCCC | 1.15 | 0.94 | 0.95 | 1.05 | | | | | 1.65 | [117] |
| 983 | OC1CCCCCC1 | C1CCCCC1 | 0.96 | 0.79 | 0.78 | 0.90 | | | | | 1.15 | [117] |
| 984 | OC1CCCCCC1 | CC1CCCC1 | 0.98 | 0.79 | 0.78 | 0.76 | | | | | 1.21 | [117] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 985 | OC1CCCCCC1 | c1ccccc1 | 0.62 | 0.59 | 0.57 | 0.79 | | | | | 0.95 | [117] |
| 986 | C1CCCCC1 | CCCCCCC | -0.01 | 0.01 | -0.01 | 0.07 | 0.46 | -0.05 | -0.03 | 0.12 | 0.11 | [125 , 54 , 128 , 128 , 130] |
| 987 | C1CCCCC1 | CCCCC | 0.02 | 0.05 | 0.00 | 0.11 | 0.40 | -0.03 | 0.05 | 0.26 | 0.20 | [54] |
| 988 | C1CCCCC1 | C1CCCC1 | 0.00 | -0.02 | -0.01 | -0.01 | 0.21 | -0.21 | -0.22 | -0.03 | -0.01 | [126] |
| 989 | C1CCCCC1 | CCCCCC | 0.01 | 0.04 | 0.00 | 0.10 | 0.43 | -0.03 | 0.01 | 0.18 | 0.18 | [54 , 61 , 128 , 128] |
| 990 | C1CCCCC1 | CCCC(C)C | 0.01 | 0.04 | 0.00 | 0.10 | 0.49 | | | 0.30 | 0.18 | [54 , 61] |
| 991 | C1CCCCC1 | CC(C)C(C)C | 0.01 | 0.04 | 0.00 | 0.10 | 0.40 | | | 0.32 | 0.16 | [129] |
| 992 | C1CCCCC1 | CC(C)CC(C)C | 0.00 | 0.00 | -0.01 | 0.07 | 0.54 | | | 0.34 | 0.17 | [54 , 61] |
| 993 | C1CCCCC1 | CC1CCCCC1 | 0.00 | -0.01 | -0.01 | 0.00 | 0.16 | -0.13 | -0.13 | 0.03 | 0.02 | [131] |
| 994 | C1CCCCC1 | CCCCCCCC | -0.03 | -0.04 | -0.03 | 0.05 | 0.54 | -0.04 | -0.04 | 0.07 | 0.09 | [54 , 61 , 61 , 128 , 128] |
| 995 | C1CCCCC1 | CC(C)C(C)C(C)C | -0.02 | -0.04 | -0.03 | 0.05 | 0.27 | | | | 0.14 | [54 , 61] |
| 996 | C1CCCCC1 | CC(C)CCC(C)C | -0.02 | -0.04 | -0.03 | 0.05 | | | | | 0.18 | [54] |
| 997 | C1CCCCC1 | CCC1CCCCC1 | -0.02 | -0.04 | -0.02 | -0.01 | | | | 0.00 | 0.06 | [54 , 61] |
| 998 | C1CCCCC1 | CCCCCCCCC | -0.06 | -0.11 | -0.05 | 0.03 | 0.69 | -0.04 | -0.04 | 0.00 | 0.03 | [54 , 61 , 128] |
| 999 | C1CCCCC1 | CCCCCCCCCC | -0.09 | -0.17 | -0.08 | 0.00 | 0.82 | -0.03 | -0.03 | -0.06 | -0.08 | [128] |
| 1000 | C1CCCCC1 | CCCCCCCCCCCC | -0.16 | -0.34 | -0.15 | -0.06 | 0.55 | -0.03 | -0.04 | -0.22 | -0.12 | [128] |
| 1001 | C1CCCCC1 | CCCCCCCCCCCCCC | -0.25 | -0.53 | -0.22 | -0.12 | 0.69 | -0.03 | -0.04 | -0.39 | -0.19 | [128] |
| 1002 | C1CCCCC1 | c1ccccc1 | 0.50 | 0.40 | 0.39 | 0.49 | 0.77 | -0.17 | -0.12 | 0.45 | 0.48 | [61 , 78 , 108] |
| 1003 | C1CCCCC1 | Cc1ccccc1 | 0.49 | 0.40 | 0.37 | 0.43 | 0.72 | -0.13 | -0.12 | 0.41 | 0.49 | [61 , 65 , 78] |
| 1004 | C1CCCCC1 | Cc1cccc(C)c1 | 0.41 | 0.33 | 0.31 | 0.37 | 0.76 | -0.06 | -0.09 | | 0.46 | [130] |
| 1005 | C1CCCCC1 | CO | 4.56 | 3.20 | 3.23 | 4.26 | 4.64 | 1.02 | 6.58 | 5.35 | 4.26 | [61] |
| 1006 | C1CCCCC1 | CCO | 4.34 | 3.52 | 3.26 | 4.27 | 4.19 | 1.19 | 3.72 | 4.65 | 4.15 | [61] |
| 1007 | C1CCCCC1 | CC(C)O | 3.80 | 3.28 | 3.04 | 3.87 | 3.82 | 1.11 | 1.71 | 4.11 | 3.49 | [61] |
| 1008 | C1CCCCC1 | CCCCO | 3.92 | 3.06 | 2.85 | 3.94 | 3.78 | 1.30 | 1.55 | 4.13 | 3.74 | [61] |
| 1009 | C1CCCCC1 | CCCCCO | 3.97 | 2.86 | 2.68 | 3.80 | 3.73 | 1.28 | 0.95 | 4.06 | 3.52 | [61] |
| 1010 | C1CCCCC1 | CCC(C)(C)O | 3.21 | 2.89 | 2.66 | 3.38 | | 1.23 | 0.64 | | 2.27 | [87] |
| 1011 | C1CCCCC1 | C1COCCO1 | 1.20 | 2.19 | 1.73 | 1.41 | 1.40 | 0.12 | 0.33 | 1.42 | 1.43 | [61] |
| 1012 | C1CCCCC1 | CCOC(C)(C)C | 0.32 | 0.28 | 0.20 | 0.16 | | | | | 0.26 | [132] |
| 1013 | C1CCCCC1 | CCC(C)=O | 1.74 | 1.77 | 1.71 | 2.06 | 1.89 | 0.34 | -0.02 | 1.64 | 1.66 | [61] |
| 1014 | C1CCCCC1 | CCCC=O | 1.37 | 1.50 | 1.44 | 1.62 | 1.72 | 0.25 | -0.25 | 1.29 | 1.46 | [71] |
| 1015 | C1CCCCC1 | CCCCC=O | 1.25 | 1.36 | 1.30 | 1.52 | | 0.59 | 0.05 | | 1.25 | [71] |
| 1016 | C1CCCCC1 | CCCCCl | 0.49 | 0.22 | 0.18 | 0.39 | 0.76 | 0.02 | -0.19 | 0.54 | 0.49 | [61] |
| 1017 | C1CCCCC1 | CCSC | 0.62 | 0.59 | 0.57 | 0.55 | | | | | 0.77 | [133 , 134] |
| 1018 | C1CCCCC1 | CCSCC | 0.61 | 0.34 | 0.30 | 0.30 | | | | | 0.57 | [133 , 134] |
| 1019 | C1CCCCC1 | CCCSCCC | 0.42 | 0.22 | 0.22 | 0.29 | | | | | 0.52 | [133 , 134] |
| 1020 | C1CCCCC1 | CSSC | 0.98 | | | 0.47 | | | | | 0.84 | [133 , 134] |
| 1021 | C1CCCCC1 | CCSSCC | 0.78 | 0.99 | 0.98 | -0.14 | | | | | 0.81 | [133 , 134] |
| 1022 | C1CCCCC1 | CCCSSCCC | 0.60 | 0.72 | 0.76 | -0.48 | | | | | 0.57 | [133] |
| 1023 | OC1CCCCC1 | CCCCC | 1.17 | 0.93 | 0.94 | 1.17 | | 1.45 | 4.34 | | 1.70 | [117] |
| 1024 | OC1CCCCC1 | C1CCCC1 | 0.98 | 0.75 | 0.75 | 0.89 | | 0.67 | 2.71 | | 1.21 | [117] |
| 1025 | OC1CCCCC1 | CCCCCC | 1.34 | 1.11 | 1.11 | 1.27 | | 1.63 | 4.03 | | 1.83 | [117] |
| 1026 | OC1CCCCC1 | C1CCCCC1 | 1.14 | 0.96 | 0.93 | 1.10 | | 1.09 | 2.54 | | 1.27 | [117] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1027 | OC1CCCCC1 | CC1CCCC1 | 1.15 | 0.96 | 0.92 | 0.94 | | | | | 1.34 | [61 , 117] |
| 1028 | OC1CCCCC1 | c1ccccc1 | 1.03 | 0.72 | 0.66 | 0.94 | | 0.58 | 1.44 | | 1.03 | [117] |
| 1029 | O=C1CCCCC1 | CCCCC | 1.07 | 0.76 | 0.72 | 0.99 | 1.29 | 0.59 | 1.24 | 0.70 | 1.26 | [54 , 61 , 61 , 47] |
| 1030 | O=C1CCCCC1 | CCC(C)C | 1.02 | 0.76 | 0.71 | 0.99 | | 0.78 | 1.65 | | 1.21 | [61 , 47] |
| 1031 | O=C1CCCCC1 | CCCCCC | 1.23 | 0.87 | 0.83 | 1.07 | 1.39 | 0.64 | 1.08 | 0.78 | 1.50 | [54 , 61 , 61 , 135 , 47] |
| 1032 | O=C1CCCCC1 | C1CCCCC1 | 1.03 | 0.70 | 0.70 | 1.02 | 1.11 | 0.26 | 0.33 | 0.83 | 1.03 | [54 , 61 , 61 , 47 , 136] |
| 1033 | O=C1CCCCC1 | CCCC(C)C | 1.18 | 0.86 | 0.83 | 1.07 | 1.43 | | | 0.79 | 1.40 | [54 , 61 , 61] |
| 1034 | O=C1CCCCC1 | CCCCCCC | 1.37 | 0.96 | 0.94 | 1.14 | 1.49 | 0.68 | 0.92 | 0.86 | 1.53 | [54 , 61 , 61 , 136] |
| 1035 | O=C1CCCCC1 | CC(C)CC(C)C | 1.28 | 0.95 | 0.94 | 1.14 | 1.52 | | | 0.86 | 1.50 | [54 , 61 , 61] |
| 1036 | O=C1CCCCC1 | CCCCCCCC | 1.52 | 1.03 | 1.04 | 1.21 | 1.63 | 0.75 | 0.86 | 0.93 | 1.64 | [54 , 61 , 61 , 61] |
| 1037 | O=C1CCCCC1 | CC(C)C(C)C(C)C | 1.34 | 1.02 | 1.04 | 1.21 | 1.34 | | | | 1.51 | [54 , 61 , 61] |
| 1038 | O=C1CCCCC1 | CC(C)CCC(C)C | 1.44 | 1.02 | 1.04 | 1.21 | | | | | 1.63 | [54] |
| 1039 | O=C1CCCCC1 | CCC1CCCCC1 | 1.29 | 0.90 | 0.92 | 1.12 | | | | 0.99 | 1.36 | [54 , 61 , 61] |
| 1040 | O=C1CCCCC1 | CCCCCCCCC | 1.65 | 1.09 | 1.13 | 1.29 | 1.85 | 0.81 | 0.79 | 1.00 | 1.80 | [54 , 61 , 61] |
| 1041 | O=C1CCCCC1 | CCC(C)CCC(C)C | 1.56 | 1.08 | 1.13 | 1.29 | | | | | 1.53 | [61] |
| 1042 | O=C1CCCCC1 | c1ccccc1 | 0.00 | -0.17 | -0.19 | -0.09 | 0.15 | 0.04 | -0.11 | 0.01 | -0.12 | [61 , 47 , 136] |
| 1043 | O=C1CCCCC1 | Cc1ccccc1 | 0.18 | -0.26 | -0.30 | 0.02 | 0.16 | 0.03 | 0.00 | 0.10 | 0.01 | [61] |
| 1044 | O=C1CCCCC1 | CCCC=C | 0.58 | 0.44 | 0.41 | 0.64 | 1.11 | 0.39 | 1.24 | 0.48 | 0.94 | [61] |
| 1045 | O=C1CCCCC1 | CC=C(C)C | 0.57 | 0.60 | 0.52 | 0.70 | | 0.25 | 1.00 | | 0.74 | [47] |
| 1046 | O=C1CCCCC1 | CC(C)C=C | 0.57 | 0.44 | 0.41 | 0.64 | | | | | 0.87 | [61] |
| 1047 | O=C1CCCCC1 | CC(=C)C=C | 0.29 | 0.26 | 0.25 | 0.30 | 0.76 | | | | 0.34 | [61 , 47] |
| 1048 | O=C1CCCCC1 | CCO | 0.36 | 1.18 | 0.94 | 0.95 | 1.14 | 0.42 | 1.24 | 2.06 | 0.72 | [61] |
| 1049 | O=C1CCCCC1 | CCOC(=O)C | 0.03 | 0.17 | 0.10 | 0.11 | 0.29 | -0.13 | -0.16 | 0.23 | 0.23 | [61] |
| 1050 | O=C1CCCCC1 | C1COCCO1 | 0.08 | 0.80 | 0.36 | 0.05 | -0.34 | -0.08 | -0.25 | 0.27 | 0.04 | [61] |
| 1051 | O=C1CCCCC1 | CC(C)=O | 0.10 | 0.18 | 0.16 | 0.13 | 0.27 | -0.11 | -0.29 | 0.32 | 0.23 | [61] |
| 1052 | O=C1CCCCC1 | CCC(C)=O | 0.02 | 0.12 | 0.08 | 0.08 | 0.15 | -0.12 | -0.16 | 0.12 | 0.00 | [61] |
| 1053 | O=C1CCCCC1 | CCCCl | -0.06 | 0.05 | 0.03 | -0.01 | 0.24 | | | | 0.06 | [61] |
| 1054 | O=C1CCCCC1 | CC(C)(C)Cl | 0.00 | 0.39 | 0.34 | 0.39 | 0.53 | | | | 0.26 | [61] |
| 1055 | O=C1CCCCC1 | ClCCl | -1.08 | -0.58 | -0.53 | -0.56 | -0.73 | -0.34 | -0.34 | -0.58 | -0.92 | [61] |
| 1056 | O=C1CCCCC1 | ClC(Cl)Cl | -1.08 | -0.69 | -0.67 | -0.97 | -0.92 | -0.21 | | -1.17 | -1.14 | [61] |
| 1057 | O=C1CCCCC1 | ClC(Cl)(Cl)Cl | 0.65 | 0.23 | 0.21 | 0.19 | 0.30 | 0.14 | 0.05 | 0.04 | 0.10 | [61] |
| 1058 | O=C1CCCCC1 | CCBr | -0.22 | 0.00 | 0.01 | -0.04 | 0.26 | -0.21 | | | -0.04 | [61] |
| 1059 | O=C1CCCCC1 | CCI | -0.17 | 0.31 | 0.34 | -0.53 | 0.77 | | | | 0.12 | [61] |
| 1060 | O=C1CCCCC1 | CCN(CC)CC | 0.72 | 0.51 | 0.49 | 0.94 | 1.04 | 0.31 | 0.12 | 0.47 | 0.94 | [61] |
| 1061 | O=C1CCCCC1 | C(=S)=S | 0.65 | 0.67 | 0.77 | 0.46 | | -0.04 | -0.37 | | 0.62 | [61] |
| 1062 | CC(=O)CC1CCCCC1 | CCCCC | 0.64 | 0.51 | 0.52 | 0.77 | | | | | 0.90 | [47] |
| 1063 | CC(=O)CC1CCCCC1 | CCC(C)C | 0.60 | 0.51 | 0.52 | 0.77 | | | | | 0.82 | [47] |
| 1064 | CC(=O)CC1CCCCC1 | CCCCCC | 0.75 | 0.65 | 0.64 | 0.84 | | | | | 0.95 | [47] |
| 1065 | CC(=O)CC1CCCCC1 | C1CCCCC1 | 0.60 | 0.48 | 0.52 | 0.77 | | | | | 0.73 | [47] |
| 1066 | CC(=O)CC1CCCCC1 | c1ccccc1 | -0.11 | -0.37 | -0.30 | -0.22 | | | | | -0.03 | [47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1067 | CC(=O)CC1CCCCC1 | CC=C(C)C | 0.25 | 0.36 | 0.34 | 0.49 | | | | | 0.58 | [47] |
| 1068 | CC(=O)CC1CCCCC1 | CC(=C)C=C | 0.06 | 0.03 | 0.10 | 0.13 | | | | | 0.28 | [47] |
| 1069 | NC1CCCCC1 | CCCCCCC | 0.87 | 0.45 | 0.43 | 0.83 | | 0.45 | 0.38 | | 0.85 | [137] |
| 1070 | C1CCC(CC1)c2ccccc2 | CCCCCC | 0.34 | 0.25 | 0.10 | 0.46 | | | | | 0.47 | [118] |
| 1071 | C1CCC(CC1)c2ccccc2 | C1CCCCC1 | 0.20 | 0.04 | 0.05 | 0.26 | | | | | 0.21 | [118] |
| 1072 | C1CCC(CC1)c2ccccc2 | CCCCCCC | 0.38 | 0.31 | 0.13 | 0.47 | | | | | 0.48 | [118] |
| 1073 | C1CCC(CC1)c2ccccc2 | c1ccccc1 | -0.08 | -0.12 | 0.00 | -0.04 | | | | | -0.03 | [118] |
| 1074 | C1CCC(CC1)c2ccccc2 | CCCCC=C | 0.13 | 0.15 | 0.02 | 0.32 | | | | | 0.28 | [118] |
| 1075 | C1CCC(CC1)c2ccccc2 | C1CCC=CC1 | 0.02 | -0.05 | -0.02 | 0.04 | | | | | 0.04 | [118] |
| 1076 | C1CCC(CC1)c2ccccc2 | C1CC=CC=C1 | -0.04 | -0.29 | -0.07 | 0.05 | | | | | -0.05 | [118] |
| 1077 | C1CCC(CC1)c2ccccc2 | C1C=CCC=C1 | -0.04 | -0.29 | -0.07 | 0.05 | | | | | -0.15 | [118] |
| 1078 | C1CCC(CC1)c2ccccc2 | CCCCCC=C | 0.17 | 0.21 | 0.05 | 0.34 | | | | | 0.30 | [118] |
| 1079 | C1CCC(CC1)c2ccccc2 | CCCCC#C | 0.08 | 0.61 | 0.43 | -0.30 | | | | | 0.17 | [118] |
| 1080 | C1CCC(CC1)c2ccccc2 | CCCCCC#C | 0.09 | 0.57 | 0.36 | -0.33 | | | | | 0.17 | [118] |
| 1081 | C1CCCCCCC1 | CCCCCCC | 0.04 | 0.04 | 0.00 | 0.06 | | 0.03 | 0.14 | 0.30 | 0.26 | [125] |
| 1082 | C1CCCCCCC1 | C1CCCC1 | -0.02 | -0.09 | -0.04 | -0.05 | | -0.25 | -0.22 | -0.05 | -0.01 | [138] |
| 1083 | C1CCCCCCC1 | C1CCCCC1 | 0.00 | -0.04 | -0.02 | -0.02 | | -0.24 | -0.21 | -0.03 | 0.05 | [126] |
| 1084 | C1CCCCCCC1 | CC(C)C(C)C | 0.04 | 0.03 | -0.01 | 0.05 | | | | 0.50 | 0.29 | [139] |
| 1085 | C1CCCCCCC1 | c1ccccc1 | 0.40 | 0.31 | 0.34 | 0.40 | | -0.29 | -0.29 | 0.41 | 0.29 | [65] |
| 1086 | C1CCCCCCC1 | Cc1ccccc1 | 0.41 | 0.35 | 0.35 | 0.35 | | -0.22 | -0.25 | 0.39 | 0.51 | [65] |
| 1087 | C1CCCC1 | CCCCCCC | -0.04 | -0.07 | -0.04 | 0.06 | | -0.03 | -0.05 | 0.04 | 0.09 | [125] |
| 1088 | C1CCCC1 | c1ccccc1 | 0.51 | 0.43 | 0.40 | 0.54 | | -0.12 | -0.05 | 0.49 | 0.51 | [78] |
| 1089 | OC1CCCC1 | CCCCC | 1.32 | 1.13 | 1.13 | 1.46 | | | | | 1.78 | [117] |
| 1090 | OC1CCCC1 | C1CCCC1 | 1.13 | 0.94 | 0.91 | 1.14 | | | | | 1.41 | [117] |
| 1091 | OC1CCCC1 | CCCCCC | 1.50 | 1.32 | 1.32 | 1.57 | | | | | 1.88 | [117] |
| 1092 | OC1CCCC1 | C1CCCCC1 | 1.29 | 1.16 | 1.11 | 1.38 | | | | | 1.43 | [117] |
| 1093 | OC1CCCC1 | CC1CCCC1 | 1.31 | 1.16 | 1.11 | 1.20 | | | | | 1.49 | [117] |
| 1094 | OC1CCCC1 | c1ccccc1 | 0.87 | 0.87 | 0.77 | 1.12 | | | | | 1.10 | [117] |
| 1095 | O=C1CCCC1 | CCCCC | 1.32 | 0.96 | 0.92 | 1.28 | | 1.36 | 1.93 | | 1.57 | [74] |
| 1096 | O=C1CCCC1 | C1CCCCC1 | 1.27 | 0.89 | 0.90 | 1.30 | | 0.97 | 0.86 | | 1.36 | [136] |
| 1097 | O=C1CCCC1 | CCCCCCC | 1.67 | 1.16 | 1.18 | 1.47 | | 1.64 | 1.56 | | 1.75 | [136] |
| 1098 | O=C1CCCC1 | c1ccccc1 | 0.07 | -0.05 | -0.08 | 0.01 | | 0.63 | 0.27 | | 0.05 | [136] |
| 1099 | O=C1CCCC1 | CCCC=C | 0.71 | 0.61 | 0.58 | 0.86 | | 1.02 | 1.94 | | 1.07 | [74] |
| 1100 | NC1CCCC1 | CCCCCCC | 1.09 | 0.53 | 0.52 | 1.12 | | | | | 0.72 | [137] |
| 1101 | C1CCC2CCCCC2C1 | CCCCCC | 0.03 | 0.09 | -0.02 | 0.26 | | | 0.36 | 0.35 | 0.25 | [59 , 59 , 118 , 47 , 140 , 140 , 140 , 140 , 140] |
| 1102 | C1CCC2CCCCC2C1 | C1CCCCC1 | -0.02 | -0.06 | -0.04 | 0.05 | | | -0.21 | -0.05 | 0.07 | [118 , 47 , 61 , 140 , 140 , 140 , 140 , 140] |
| 1103 | C1CCC2CCCCC2C1 | CCCCCCC | 0.04 | 0.11 | -0.01 | 0.26 | | | 0.25 | 0.33 | 0.25 | [118 , 140 , 140 , 140] |
| 1104 | C1CCC2CCCCC2C1 | c1ccccc1 | 0.36 | 0.22 | 0.31 | 0.34 | | | -0.36 | 0.36 | 0.37 | [59 , 118 , 47 , 61 , 140 , 140 , 140 , 140] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1105 | C1CCC2CCCCC2C1 | CCCCC=C | 0.06 | 0.12 | 0.04 | 0.31 | | | 0.42 | 0.25 | 0.28 | [118] |
| 1106 | C1CCC2CCCCC2C1 | C1CCC=CC1 | 0.00 | -0.04 | 0.00 | 0.02 | | | -0.33 | | 0.07 | [118] |
| 1107 | C1CCC2CCCCC2C1 | C1CC=CC=C1 | 0.12 | -0.11 | 0.09 | 0.24 | | | | | 0.10 | [118] |
| 1108 | C1CCC2CCCCC2C1 | C1C=CCC=C1 | 0.13 | -0.11 | 0.09 | 0.24 | | | | | 0.05 | [118] |
| 1109 | C1CCC2CCCCC2C1 | CCCCCC=C | 0.06 | 0.16 | 0.05 | 0.32 | | | 0.25 | | 0.24 | [118] |
| 1110 | C1CCC2CCCCC2C1 | CCCCC#C | 0.44 | 1.39 | 1.26 | -0.39 | | | | | 0.57 | [118] |
| 1111 | C1CCC2CCCCC2C1 | CCCCCC#C | 0.40 | 1.31 | 1.18 | -0.42 | | | | | 0.55 | [118] |
| 1112 | C1CCC2CCCCC2C1 | CCCCC | 0.02 | 0.03 | -0.05 | 0.25 | | | 0.49 | 0.41 | 0.29 | [140 , 140 , 140 , 140 , 140] |
| 1113 | C1CCC2CCCCC2C1 | C1CCCC1 | -0.04 | -0.14 | -0.07 | -0.01 | | | -0.21 | -0.09 | 0.00 | [140 , 140 , 140 , 140 , 140] |
| 1114 | C1CCC2CCCCC2C1 | CC=C(C)C | 0.00 | 0.10 | -0.03 | 0.20 | | | 0.28 | | 0.19 | [47 , 61] |
| 1115 | C1CCC2CCCCC2C1 | CC(=C)C=C | 0.24 | 0.13 | 0.13 | 0.25 | | | | | 0.31 | [61 , 47] |
| 1116 | O=[S]1(=O)CC(CC1)OCCCCCCCCCC | CCCCCC | 1.06 | 0.77 | 0.89 | 1.24 | | | | | 1.48 | [73] |
| 1117 | O=[S]1(=O)CC(CC1)OCCCCCCCCCC | c1ccccc1 | -0.09 | -0.40 | -0.16 | -0.27 | | | | | 0.00 | [73] |
| 1118 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCC | 0.08 | -0.31 | -0.04 | 0.17 | | | | | 0.35 | [121] |
| 1119 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCCC | 0.17 | -0.15 | 0.08 | 0.26 | | | | | 0.45 | [121] |
| 1120 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | C1CCCCC1 | 0.05 | -0.34 | -0.02 | 0.15 | | | | | 0.10 | [121] |
| 1121 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCCCC | 0.26 | -0.01 | 0.17 | 0.35 | | | | | 0.54 | [121] |
| 1122 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CC1CCCCC1 | 0.13 | -0.17 | 0.09 | 0.20 | | | | | 0.19 | [121] |
| 1123 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCCCCC | 0.34 | 0.11 | 0.26 | 0.44 | | | | | 0.63 | [121] |
| 1124 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCC1CCCCC1 | 0.22 | -0.04 | 0.18 | 0.30 | | | | | 0.28 | [121] |
| 1125 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | c1ccccc1 | -0.31 | -0.84 | -0.46 | -0.65 | | | | | -0.39 | [121] |
| 1126 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | Cc1ccccc1 | -0.20 | -0.73 | -0.43 | -0.58 | | | | | -0.29 | [121] |
| 1127 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCc1ccccc1 | -0.15 | -0.58 | -0.34 | -0.45 | | | | | -0.25 | [121] |
| 1128 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCC=C | -0.19 | -0.54 | -0.24 | -0.17 | | | | | 0.04 | [121] |
| 1129 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCC=C | -0.09 | -0.39 | -0.13 | -0.06 | | | | | 0.19 | [121] |
| 1130 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCCC=C | -0.02 | -0.24 | -0.03 | 0.04 | | | | | 0.34 | [121] |
| 1131 | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | CCCCCCC=C | 0.07 | -0.12 | 0.06 | 0.13 | | | | | 0.45 | [121] |
| 1132 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCC | 0.60 | 0.29 | 0.43 | 0.65 | | 0.44 | 1.68 | | 0.54 | [121] |
| 1133 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCC | 0.75 | 0.49 | 0.59 | 0.78 | | 0.54 | 1.37 | | 0.66 | [121] |
| 1134 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | C1CCCCC1 | 0.54 | 0.26 | 0.44 | 0.64 | | 0.08 | -0.01 | | 0.27 | [121] |
| 1135 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCC | 0.88 | 0.66 | 0.73 | 0.90 | | 0.64 | 1.08 | | 0.78 | [121] |
| 1136 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CC1CCCCC1 | 0.66 | 0.45 | 0.59 | 0.71 | | 0.29 | 0.49 | | 0.38 | [121] |
| 1137 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCCC | 1.00 | 0.82 | 0.86 | 1.02 | | 0.75 | 0.97 | | 0.91 | [121] |
| 1138 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCC1CCCCC1 | 0.78 | 0.63 | 0.72 | 0.84 | | | | | 0.50 | [121] |
| 1139 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | c1ccccc1 | -0.22 | -0.56 | -0.33 | -0.42 | | -0.21 | -0.62 | | -0.54 | [121] |
| 1140 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | Cc1ccccc1 | -0.05 | -0.48 | -0.30 | -0.29 | | -0.17 | -0.46 | | -0.36 | [121] |
| 1141 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCc1ccccc1 | 0.04 | -0.26 | -0.14 | -0.13 | | 0.06 | -0.33 | | -0.19 | [121] |
| 1142 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCC=C | 0.19 | -0.02 | 0.15 | 0.22 | | 0.22 | 1.67 | | 0.15 | [121] |
| 1143 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCC=C | 0.34 | 0.17 | 0.29 | 0.36 | | 0.39 | 1.50 | | 0.27 | [121] |
| 1144 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCC=C | 0.45 | 0.34 | 0.43 | 0.49 | | 0.36 | 1.10 | | 0.40 | [121] |
| 1145 | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | CCCCCCC=C | 0.59 | 0.49 | 0.55 | 0.62 | | 0.41 | 0.92 | | 0.52 | [121] |
| 1146 | CCCCNCCCC | CCCCCCC | 0.27 | 0.16 | 0.17 | 0.28 | | | | | 0.19 | [137] |
| 1147 | C(C(=O)O)(Cl)Cl | CCCCCC | 2.56 | 3.31 | 3.34 | 2.83 | | 1.97 | 2.32 | | 2.67 | [47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1148 | C(C(=O)O)(Cl)Cl | C1CCCCC1 | 2.13 | 2.85 | 2.81 | 2.72 | | 1.31 | 1.33 | | 2.18 | [47] |
| 1149 | C(C(=O)O)(Cl)Cl | c1ccccc1 | 1.17 | 0.85 | 0.73 | 0.53 | | 0.76 | 0.63 | | 0.87 | [47] |
| 1150 | C(C(=O)O)(Cl)Cl | CC=C(C)C | 1.60 | 2.63 | 2.62 | 1.86 | | 0.95 | 2.25 | | 1.73 | [47] |
| 1151 | C(C(=O)O)(Cl)Cl | CC(=C)C=C | 1.40 | 2.01 | 2.01 | 0.80 | | | | | 1.33 | [47] |
| 1152 | ClCCl | c1ccccc1 | 0.11 | -0.43 | -0.54 | -0.01 | 0.42 | 0.18 | -0.08 | 0.00 | -0.08 | [141] |
| 1153 | ClCCl | Cc1ccccc1 | 0.10 | -0.37 | -0.45 | 0.03 | 0.48 | 0.17 | -0.03 | -0.01 | -0.09 | [141 , 61] |
| 1154 | ClCCl | CCCCC | 0.91 | 0.76 | 0.85 | 0.91 | 1.71 | 0.83 | 0.64 | 1.26 | 1.13 | [142 , 54 , 61 , 61] |
| 1155 | ClCCl | CCCCCC | 0.97 | 0.78 | 0.95 | 1.03 | 1.86 | 0.88 | 0.55 | 1.28 | 1.42 | [55 , 54] |
| 1156 | ClCCl | CCO | 2.02 | 1.68 | 1.58 | 2.36 | 2.58 | 0.51 | 0.95 | 2.32 | 2.22 | [61] |
| 1157 | ClCCl | C1COCCO1 | -1.31 | -0.87 | -1.02 | -1.14 | -0.65 | -0.01 | -0.12 | -0.97 | -0.87 | [61] |
| 1158 | ClCCl | CCC(C)=O | -1.39 | -0.87 | -0.84 | -0.82 | -0.01 | 0.03 | -0.11 | -0.94 | -0.82 | [61] |
| 1159 | ClCCl | CCN(CC)CC | -0.16 | -0.05 | 0.18 | -0.09 | 0.40 | 0.45 | 0.04 | -0.48 | -0.06 | [61] |
| 1160 | N#CCC#N | CCCCCC | 5.76 | | | | | | | | 5.23 | [47] |
| 1161 | N#CCC#N | C1CCCCC1 | 4.91 | | | | | | | | 4.49 | [47] |
| 1162 | N#CCC#N | c1ccccc1 | 2.34 | | | | | | | | 2.00 | [47] |
| 1163 | N#CCC#N | CC=C(C)C | 3.77 | | | | | | | | 3.66 | [47] |
| 1164 | N#CCC#N | CC(=C)C=C | 2.96 | | | | | | | | 2.88 | [47] |
| 1165 | CCOC(=O)OCC | CCCCC | 0.97 | | | 0.89 | | 0.25 | 0.39 | | 1.06 | [74] |
| 1166 | CCOC(=O)OCC | C1CCCCC1 | 0.93 | | | 0.92 | | 0.07 | -0.15 | | 1.35 | [143] |
| 1167 | CCOC(=O)OCC | c1ccccc1 | -0.02 | | | -0.03 | | -0.07 | -0.27 | | -0.09 | [143] |
| 1168 | CCOC(=O)OCC | CCCC=C | 0.49 | | | 0.56 | | 0.03 | 0.39 | | 0.65 | [74] |
| 1169 | CCOCC | C1CCCCC1 | 0.29 | 0.34 | 0.25 | 0.28 | 0.31 | 0.17 | -0.06 | 0.66 | 0.44 | [57] |
| 1170 | CCOC(=O)C(=O)OCC | CCCCC | 1.56 | 1.27 | 1.29 | 1.35 | | 0.83 | 1.47 | | 1.90 | [74] |
| 1171 | CCOC(=O)C(=O)OCC | CCCC=C | 0.93 | 0.79 | 0.82 | 0.84 | | 0.34 | 1.47 | | 1.34 | [74] |
| 1172 | CCNCC | CCCCCCC | 0.59 | 0.38 | 0.41 | 0.44 | | 0.26 | -0.07 | | 0.45 | [137] |
| 1173 | CCSSCC | C1CCCCC1 | 0.51 | 0.72 | 0.71 | -0.17 | | | | | 0.64 | [134 , 133] |
| 1174 | CCSSCC | CCCCCCC | 0.73 | 0.96 | 0.96 | 0.65 | | | | | 0.64 | [134 , 133] |
| 1175 | C(COCCO)O | CCCCCC | 3.11 | 2.89 | 2.74 | 3.95 | 4.18 | 4.49 | 3.62 | | 4.67 | [144 , 47 , 73 , 5] |
| 1176 | C(COCCO)O | C1CCCCC1 | 2.66 | 2.60 | 2.29 | 3.79 | 3.60 | 3.53 | 2.28 | | 3.93 | [144 , 5] |
| 1177 | C(COCCO)O | CCCCCCC | 3.51 | 3.33 | 3.12 | 4.39 | 4.61 | 5.03 | 3.34 | | 5.11 | [144 , 5] |
| 1178 | C(COCCO)O | CC1CCCCC1 | 3.00 | 3.06 | 2.68 | 3.97 | 3.99 | 3.99 | 2.81 | | 4.36 | [144 , 5] |
| 1179 | C(COCCO)O | CCCCCCCC | 3.89 | 3.75 | 3.50 | 4.82 | 5.08 | 5.59 | 3.21 | | 5.52 | [144 , 5] |
| 1180 | C(COCCO)O | CC(C)CC(C)(C)C | 3.49 | 3.75 | 3.55 | 4.81 | 4.64 | 5.88 | 4.29 | | 5.30 | [144 , 5] |
| 1181 | C(COCCO)O | CCC1CCCCC1 | 3.36 | 3.49 | 3.06 | 4.41 | | | | | 4.76 | [144] |
| 1182 | C(COCCO)O | CCCCCCCCC | 4.28 | 4.15 | 3.87 | 5.24 | 5.63 | 6.14 | 3.09 | | 5.94 | [144 , 5] |
| 1183 | C(COCCO)O | c1ccccc1 | 1.31 | 1.52 | 1.14 | 2.11 | 1.54 | 2.52 | 1.30 | | 1.90 | [144 , 47 , 5] |
| 1184 | C(COCCO)O | Cc1ccccc1 | 1.72 | 1.93 | 1.44 | 2.36 | 1.92 | 2.86 | 1.52 | | 2.34 | [144 , 5] |
| 1185 | C(COCCO)O | Cc1cccc(C)c1 | 2.06 | 2.27 | 1.69 | 2.61 | 2.30 | 3.13 | 1.58 | | 2.83 | [144 , 5] |
| 1186 | C(COCCO)O | Cc1ccc(C)cc1 | 2.07 | 2.27 | 1.69 | 2.61 | 2.24 | 3.09 | 1.68 | | 2.84 | [144 , 5] |
| 1187 | C(COCCO)O | Cc1ccccc1C | 1.96 | 2.27 | 1.69 | 2.61 | 2.18 | 3.05 | 1.58 | | 2.70 | [144 , 5] |
| 1188 | C(COCCO)O | CCc1ccccc1 | 2.05 | 2.39 | 1.84 | 3.10 | 2.34 | 3.63 | 1.70 | | 2.79 | [144 , 5] |
| 1189 | C(COCCO)O | CCCc1ccccc1 | 2.41 | 2.80 | 2.19 | 3.55 | 2.72 | | | | 3.25 | [144] |
| 1190 | C(COCCO)O | CC(C)c1ccccc1 | 2.31 | 2.84 | 2.23 | 3.39 | 2.67 | 4.18 | 1.56 | | 3.19 | [144] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1191 | C(COCCO)O | CCC\C=C/C | 2.44 | 2.82 | 2.66 | 3.50 | | | | | 3.92 | [144] |
| 1192 | C(COCCO)O | C1CCC=CC1 | 2.09 | 2.54 | 2.22 | 2.96 | 2.95 | 2.08 | 1.62 | | 3.24 | [144 , 5] |
| 1193 | C(COCCO)O | CCCCCC=C | 2.82 | 3.30 | 3.09 | 3.93 | 3.91 | 3.78 | 3.36 | | 4.42 | [144 , 5] |
| 1194 | C(COCCO)O | CCCCCCC=C | 3.24 | 3.72 | 3.46 | 4.37 | 4.39 | 4.13 | 3.19 | | 4.85 | [144] |
| 1195 | C(COCCO)O | CC(=C)CC(C)(C)C | 2.89 | 3.71 | 3.58 | 4.38 | | | | | 4.69 | [144] |
| 1196 | C(COCCO)O | CCCCCCCCCC | 4.66 | 4.55 | 4.24 | 5.67 | 6.16 | 6.72 | 3.10 | | 6.41 | [5] |
| 1197 | C(COCCO)O | CCCCCCCCCCC | 5.03 | 4.94 | 4.60 | 6.09 | 6.24 | | | | 6.85 | [5] |
| 1198 | C(COCCO)O | C=CCCCCC=C | 2.64 | 3.73 | 3.47 | 4.02 | | | | | 4.16 | [5] |
| 1199 | C(COCCO)O | CCCCCC#C | 1.69 | 2.66 | 2.41 | 3.14 | | | | | 2.97 | [5] |
| 1200 | C(COCCO)O | CCCCCCC#C | 2.04 | 2.99 | 2.71 | 3.54 | | | | | 3.37 | [5] |
| 1201 | C(COCCO)O | CCCCOC(=O)C | 1.34 | 1.67 | 1.53 | 1.97 | 1.87 | 2.11 | 1.97 | | 2.45 | [5] |
| 1202 | C(COCCO)O | C1CCOC1 | 0.33 | 1.20 | 1.18 | 2.61 | 0.54 | 0.75 | 0.85 | | 1.14 | [5] |
| 1203 | C(COCCO)O | CCCCCl | 1.48 | 2.08 | 1.98 | 2.50 | 2.37 | 2.29 | 1.91 | | 2.65 | [5] |
| 1204 | C(COCCO)O | ClCCl | -0.16 | 0.37 | 0.45 | 0.52 | 0.41 | 0.68 | 0.49 | | 0.45 | [5] |
| 1205 | C(COCCO)O | CC(Cl)CCl | 0.84 | 2.08 | 1.96 | 1.99 | 1.60 | | | | 1.51 | [5] |
| 1206 | C(COCCO)O | ClC(Cl)Cl | 0.12 | 0.16 | 0.09 | -0.13 | 0.48 | 1.27 | | | 0.42 | [5] |
| 1207 | C(COCCO)O | Clc1ccccc1 | 1.38 | 1.75 | 1.23 | 1.61 | 1.81 | 2.49 | 0.86 | | 1.88 | [5] |
| 1208 | C(COCCO)O | CC(C)Br | 1.04 | 1.42 | 1.36 | 2.38 | | | | | 2.19 | [5] |
| 1209 | C(COCCO)O | Brc1ccccc1 | 1.83 | 2.17 | 1.60 | 2.57 | 1.78 | 2.24 | 0.22 | | 2.00 | [5] |
| 1210 | C(COCCO)O | CC#N | 0.52 | 0.17 | 0.33 | 0.54 | 0.60 | 0.43 | -0.39 | | 0.74 | [5] |
| 1211 | C(COCCO)O | Fc1ccccc1 | 1.24 | 1.50 | 1.09 | 1.83 | | 2.09 | 0.77 | | 1.69 | [5] |
| 1212 | COCCOCCOC | C1CCCCC1 | 1.06 | 1.34 | 1.29 | 0.77 | | 0.52 | 0.08 | | 1.38 | [57] |
| 1213 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCC | 1.12 | 0.88 | 0.94 | 1.10 | | 0.68 | 2.52 | 1.47 | 1.64 | [121] |
| 1214 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCCC | 1.32 | 1.12 | 1.14 | 1.26 | | 0.80 | 2.19 | 1.64 | 1.82 | [121] |
| 1215 | CCOC(=O)c1ccccc1C(=O)OCC | C1CCCCC1 | 1.04 | 0.83 | 0.93 | 1.10 | | 0.34 | 0.70 | 1.18 | 1.39 | [121] |
| 1216 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCCCC | 1.50 | 1.34 | 1.34 | 1.43 | | 0.90 | 1.89 | 1.85 | 1.97 | [121] |
| 1217 | CCOC(=O)c1ccccc1C(=O)OCC | CC1CCCCC1 | 1.21 | 1.07 | 1.13 | 1.19 | | 0.55 | 1.27 | 1.49 | 1.56 | [121] |
| 1218 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCCCCC | 1.68 | 1.55 | 1.53 | 1.59 | | 1.03 | 1.76 | 2.06 | 2.14 | [121] |
| 1219 | CCOC(=O)c1ccccc1C(=O)OCC | CCC1CCCCC1 | 1.38 | 1.29 | 1.32 | 1.37 | | | | 1.73 | 1.74 | [121] |
| 1220 | CCOC(=O)c1ccccc1C(=O)OCC | c1ccccc1 | -0.02 | -0.30 | -0.15 | -0.19 | | 0.06 | -0.16 | -0.13 | 0.04 | [121] |
| 1221 | CCOC(=O)c1ccccc1C(=O)OCC | Cc1ccccc1 | 0.20 | -0.24 | -0.14 | 0.01 | | 0.08 | 0.04 | 0.09 | 0.20 | [121] |
| 1222 | CCOC(=O)c1ccccc1C(=O)OCC | CCc1ccccc1 | 0.34 | 0.06 | 0.11 | 0.22 | | 0.33 | 0.22 | 0.32 | 0.36 | [121] |
| 1223 | CCOC(=O)c1ccccc1C(=O)OCC | CCCC=C | 0.59 | 0.48 | 0.55 | 0.57 | | 0.42 | 2.52 | 1.03 | 1.07 | [121] |
| 1224 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCC=C | 0.78 | 0.71 | 0.76 | 0.76 | | 0.63 | 2.33 | 1.26 | 1.25 | [121] |
| 1225 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCCC=C | 0.95 | 0.93 | 0.95 | 0.93 | | 0.58 | 1.90 | | 1.45 | [121] |
| 1226 | CCOC(=O)c1ccccc1C(=O)OCC | CCCCCCC=C | 1.16 | 1.14 | 1.13 | 1.10 | | 0.64 | 1.72 | 1.53 | 1.67 | [121] |
| 1227 | CCSCC | C1CCCCC1 | 0.48 | 0.30 | 0.27 | 0.24 | | | | | 0.59 | [134 , 133] |
| 1228 | CCSCC | CCCCCCC | 0.63 | 0.31 | 0.34 | 0.29 | | | | | 0.58 | [134 , 133] |
| 1229 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCC | 0.54 | 0.30 | 0.44 | 0.65 | | | | | 0.97 | [121] |
| 1230 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCCC | 0.68 | 0.49 | 0.59 | 0.78 | | | | | 1.11 | [121] |
| 1231 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | C1CCCCC1 | 0.49 | 0.26 | 0.44 | 0.64 | | | | | 0.71 | [121] |
| 1232 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCCCC | 0.80 | 0.66 | 0.73 | 0.90 | | | | | 1.28 | [121] |
| 1233 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CC1CCCCC1 | 0.61 | 0.45 | 0.59 | 0.71 | | | | | 0.85 | [121] |
| 1234 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCCCCC | 0.92 | 0.82 | 0.86 | 1.02 | | | | | 1.45 | [121] |
| 1235 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCC1CCCCC1 | 0.73 | 0.63 | 0.72 | 0.84 | | | | | 1.00 | [121] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1236 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | c1ccccc1 | -0.19 | -0.56 | -0.33 | -0.42 | | | | | -0.15 | [121] |
| 1237 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | Cc1ccccc1 | -0.04 | -0.48 | -0.30 | -0.29 | | | | | -0.03 | [121] |
| 1238 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCc1ccccc1 | 0.05 | -0.26 | -0.14 | -0.13 | | | | | 0.06 | [121] |
| 1239 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCC=C | 0.15 | -0.02 | 0.15 | 0.22 | | | | | 0.62 | [121] |
| 1240 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCC=C | 0.28 | 0.17 | 0.29 | 0.36 | | | | | 0.74 | [121] |
| 1241 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCCC=C | 0.39 | 0.34 | 0.43 | 0.49 | | | | | 0.86 | [121] |
| 1242 | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | CCCCCCC=C | 0.53 | 0.50 | 0.55 | 0.62 | | | | | 0.95 | [121] |
| 1243 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCC | 0.02 | -0.36 | -0.08 | 0.26 | | -0.37 | 1.37 | | 0.18 | [121] |
| 1244 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCCC | 0.10 | -0.19 | 0.03 | 0.35 | | -0.29 | 0.96 | | 0.23 | [121] |
| 1245 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | C1CCCCC1 | -0.03 | -0.40 | -0.06 | 0.17 | | -0.56 | -0.63 | | -0.05 | [121] |
| 1246 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCCCC | 0.19 | -0.05 | 0.13 | 0.44 | | -0.21 | 0.61 | | 0.29 | [121] |
| 1247 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CC1CCCCC1 | 0.05 | -0.24 | 0.04 | 0.22 | | -0.43 | -0.09 | | 0.08 | [121] |
| 1248 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCCCCC | 0.26 | 0.08 | 0.22 | 0.52 | | -0.12 | 0.48 | | 0.33 | [121] |
| 1249 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCC1CCCCC1 | 0.13 | -0.09 | 0.14 | 0.32 | | | | | 0.20 | [121] |
| 1250 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | c1ccccc1 | -0.39 | -0.89 | -0.49 | -0.69 | | -0.71 | -0.92 | | -0.54 | [121] |
| 1251 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | Cc1ccccc1 | -0.27 | -0.78 | -0.45 | -0.63 | | -0.67 | -0.87 | | -0.45 | [121] |
| 1252 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCc1ccccc1 | -0.21 | -0.63 | -0.36 | -0.45 | | -0.49 | -0.78 | | -0.34 | [121] |
| 1253 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCC=C | -0.24 | -0.56 | -0.26 | -0.12 | | -0.49 | 1.36 | | 0.07 | [121] |
| 1254 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCC=C | -0.15 | -0.42 | -0.16 | -0.01 | | -0.40 | 1.12 | | 0.12 | [121] |
| 1255 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCCC=C | -0.07 | -0.27 | -0.06 | 0.10 | | -0.39 | 0.62 | | 0.16 | [121] |
| 1256 | CC(C)CCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCC(C)C | CCCCCCC=C | 0.01 | -0.14 | 0.02 | 0.18 | | -0.34 | 0.42 | | 0.20 | [121] |
| 1257 | CC(C)OC(C)C | CCCCC | 0.20 | 0.04 | 0.05 | 0.06 | 0.61 | | | 0.12 | -0.02 | [61] |
| 1258 | CC(C)OC(C)C | CCCCCC | 0.25 | 0.07 | 0.07 | 0.07 | 0.73 | | | 0.17 | 0.04 | [61] |
| 1259 | CC(C)OC(C)C | C1CCCCC1 | 0.22 | 0.10 | 0.05 | 0.09 | 0.41 | | | 0.27 | 0.15 | [61] |
| 1260 | CC(C)OC(C)C | CCCC(C)C | 0.24 | 0.07 | 0.07 | 0.07 | 0.75 | | | 0.17 | 0.05 | [61] |
| 1261 | CC(C)OC(C)C | CCCCCCC | 0.29 | 0.08 | 0.08 | 0.07 | 0.84 | | | 0.23 | 0.16 | [61] |
| 1262 | CC(C)OC(C)C | CCCCCCCC | 0.33 | 0.07 | 0.08 | 0.08 | 1.00 | | | 0.27 | 0.28 | [61 , 61] |
| 1263 | CC(C)OC(C)C | CC(C)C(C)C(C)C | 0.28 | 0.07 | 0.08 | 0.08 | 0.70 | | | | 0.22 | [61] |
| 1264 | CC(C)OC(C)C | CCC1CCCCC1 | 0.31 | 0.13 | 0.08 | 0.11 | | | | 0.36 | 0.36 | [61] |
| 1265 | CC(C)OC(C)C | CCCCCCCCC | 0.36 | 0.05 | 0.08 | 0.08 | 1.24 | | | 0.31 | 0.49 | [61] |
| 1266 | CC(C)OC(C)C | CCC(C)CCC(C)C | 0.33 | 0.05 | 0.08 | 0.08 | | | | | 0.18 | [61] |
| 1267 | CC(C)OC(C)C | Cc1ccccc1 | 0.18 | 0.25 | 0.12 | 0.21 | 0.20 | | | 0.02 | 0.22 | [61] |
| 1268 | CC(C)OC(C)C | CCO | 0.79 | 2.13 | 2.06 | 2.05 | 0.93 | | | 2.05 | 1.54 | [61] |
| 1269 | CC(C)OC(C)C | C1COCCO1 | 0.39 | 1.26 | 1.06 | 0.49 | 0.49 | | | 0.75 | 0.77 | [61] |
| 1270 | CC(C)OC(C)C | CCC(C)=O | 0.48 | 1.07 | 1.10 | 0.97 | 0.99 | | | 0.63 | 0.73 | [61] |
| 1271 | COCOC | C1CCCCC1 | 0.80 | 1.99 | 1.86 | 1.18 | | 0.42 | -0.14 | | 1.06 | [57] |
| 1272 | COC(=O)OC | C1CCCCC1 | 1.68 | | | 1.91 | | 0.60 | -0.02 | 1.60 | 2.13 | [145] |
| 1273 | COC(=O)OC | c1ccccc1 | 0.36 | | | 0.41 | | 0.41 | -0.17 | 0.25 | 0.41 | [145] |
| 1274 | CSSC | CCCCC | 0.92 | 1.98 | 1.98 | 1.10 | | | | | 0.86 | [54 , 61 , 61] |
| 1275 | CSSC | CCCCCC | 1.04 | 2.25 | 2.29 | 1.52 | | | | | 0.83 | [54 , 61 , 61] |
| 1276 | CSSC | C1CCCCC1 | 0.85 | 1.94 | 1.93 | 0.71 | | | | | 0.65 | [54 , 61 , 61 , 134 , 133] |
| 1277 | CSSC | CCCC(C)C | 1.01 | 2.25 | 2.28 | 1.52 | | | | | 0.87 | [54] |
| 1278 | CSSC | CCCCCCC | 1.14 | 2.51 | 2.58 | 1.95 | | | | | 0.92 | [54 , 61 , 61 , 134 , 133] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1279 | CSSC | CC(C)CC(C)C | 1.08 | 2.50 | 2.58 | 1.95 | | | | | 0.98 | [54 , 61 , 61] |
| 1280 | CSSC | CCCCCCCC | 1.25 | 2.74 | 2.87 | 2.38 | | | | | 0.75 | [54 , 61 , 61 , 61] |
| 1281 | CSSC | CC(C)C(C)C(C)C | 1.09 | 2.74 | 2.86 | 2.38 | | | | | 0.88 | [54 , 61 , 61] |
| 1282 | CSSC | CC(C)CCC(C)C | 1.21 | 2.74 | 2.87 | 2.38 | | | | | 0.92 | [54] |
| 1283 | CSSC | CCC1CCCCC1 | 1.04 | 2.47 | 2.52 | 1.59 | | | | | 0.54 | [54 , 61 , 61] |
| 1284 | CSSC | CCCCCCCCC | 1.34 | 2.97 | 3.16 | 2.81 | | | | | 0.72 | [54 , 61 , 61] |
| 1285 | CSSC | CCC(C)CCC(C)C | 1.27 | 2.96 | 3.15 | 2.81 | | | | | 0.85 | [61] |
| 1286 | CSSC | Cc1ccccc1 | -0.14 | 0.13 | 0.04 | -3.91 | | | | | 0.53 | [61 , 95] |
| 1287 | CCN(C)C | C1CCCCC1 | 0.16 | 0.17 | 0.12 | 0.49 | | | | | 1.20 | [146] |
| 1288 | CCN(C)C | CCCCCCC | 0.17 | 0.10 | 0.14 | 0.08 | | | | | 1.10 | [146] |
| 1289 | C[S](C)=O | CCCCC | 3.69 | 3.26 | 3.29 | 3.98 | 3.94 | 2.93 | 6.52 | 3.87 | 3.81 | [114 , 114 , 54 , 61 , 61] |
| 1290 | C[S](C)=O | CCCCCC | 4.24 | 3.73 | 3.80 | 4.35 | 4.32 | 3.26 | 6.19 | 4.24 | 4.34 | [114 , 114 , 114 , 147 , 59 , 59 , 47 , 54 , 61 , 61] |
| 1291 | C[S](C)=O | C1CCCCC1 | 3.63 | 3.23 | 3.20 | 2.56 | 3.76 | 2.37 | 4.66 | 3.54 | 3.63 | [114 , 114 , 147 , 47 , 54 , 61 , 61] |
| 1292 | C[S](C)=O | CCCCCCC | 4.78 | 4.17 | 4.30 | 4.71 | 4.68 | 3.58 | 5.87 | 4.65 | 4.78 | [114 , 114 , 147 , 148 , 54 , 61 , 61] |
| 1293 | C[S](C)=O | C1CCCCCC1 | 4.03 | 3.69 | 3.71 | 2.97 | 4.05 | | | 3.95 | 4.16 | [147] |
| 1294 | C[S](C)=O | CCCCCCCC | 5.31 | 4.60 | 4.79 | 5.07 | 5.10 | 3.94 | 5.72 | 5.05 | 5.13 | [114 , 147 , 54 , 61 , 61 , 61] |
| 1295 | C[S](C)=O | C1CCCCCCC1 | 4.37 | 4.14 | 4.20 | 3.36 | 4.40 | 2.98 | 4.05 | 4.36 | 4.34 | [147] |
| 1296 | C[S](C)=O | CCCCCCCCC | 5.84 | 5.02 | 5.28 | 5.43 | 5.59 | 4.30 | 5.56 | 5.45 | 5.58 | [114 , 54 , 61 , 61] |
| 1297 | C[S](C)=O | c1ccccc1 | 1.27 | 1.16 | 1.02 | 1.20 | 1.41 | 1.67 | 3.44 | 0.90 | 1.20 | [47 , 73 , 148] |
| 1298 | C[S](C)=O | CC=C(C)C | 2.67 | 2.88 | 2.89 | 3.14 | | 1.91 | 6.11 | | 3.00 | [61] |
| 1299 | C[S](C)=O | CC(=C)C=C | 1.76 | 1.99 | 2.00 | 1.34 | 2.59 | | | | 2.16 | [61] |
| 1300 | C[S](C)=O | CCCCC=C | 3.22 | 3.03 | 3.09 | 3.32 | 3.78 | 2.91 | 6.32 | 3.39 | 3.74 | [147] |
| 1301 | C[S](C)=O | CCCCCC=C | 3.71 | 3.48 | 3.58 | 3.69 | 4.08 | 2.81 | 5.90 | | 4.20 | [147] |
| 1302 | C[S](C)=O | CCCCCCC=C | 4.31 | 3.91 | 4.07 | 4.07 | 4.50 | 3.01 | 5.69 | 3.97 | 4.49 | [147] |
| 1303 | C[S](C)=O | CCCCC#C | 1.25 | 1.26 | 1.38 | 3.03 | | | | | 1.79 | [147] |
| 1304 | C[S](C)=O | CCCCCC#C | 1.78 | 1.60 | 1.78 | 3.36 | | | | | 2.23 | [147] |
| 1305 | C[S](C)=O | CCCCCCC#C | 2.30 | 1.93 | 2.19 | 3.69 | | | | | 2.54 | [147] |
| 1306 | C[S](C)=O | CCCC(C)C | 4.10 | 3.72 | 3.79 | 4.35 | 4.26 | | | 4.35 | 4.11 | [54 , 61 , 61] |
| 1307 | C[S](C)=O | CC(C)CC(C)C | 4.47 | 4.17 | 4.29 | 4.71 | 4.51 | | | 4.86 | 4.57 | [54 , 61 , 61] |
| 1308 | C[S](C)=O | CC1CCCCC1 | 4.09 | 3.69 | 3.70 | 2.91 | 4.13 | 2.82 | 5.27 | 4.08 | 3.99 | [61] |
| 1309 | C[S](C)=O | CC(C)C(C)C(C)C | 4.73 | 4.59 | 4.78 | 5.07 | 4.70 | | | | 4.75 | [54 , 61 , 61] |
| 1310 | C[S](C)=O | CC(C)CCC(C)C | 5.06 | 4.60 | 4.78 | 5.07 | | | | | 5.03 | [54] |
| 1311 | C[S](C)=O | CCC1CCCCC1 | 4.59 | 4.13 | 4.20 | 3.29 | | | | 4.53 | 4.40 | [54 , 61 , 61] |
| 1312 | C[S](C)=O | CCC(C)CCC(C)C | 5.52 | 5.01 | 5.27 | 5.43 | | | | | 4.96 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1313 | C[S](C)=O | CCO | -1.05 | -0.94 | -1.05 | -0.53 | 0.16 | 0.35 | 0.04 | -0.99 | -0.63 | [61] |
| 1314 | C[S](C)=O | COC=O | 0.00 | -0.07 | -0.08 | 0.60 | | | | | 0.57 | [148] |
| 1315 | C[S](C)=O | CCOC(=O)C | 0.85 | 1.14 | 1.15 | 1.17 | 1.29 | 0.44 | 3.30 | 0.77 | 1.39 | [148] |
| 1316 | C[S](C)=O | C1CCOC1 | 1.25 | 1.47 | 1.48 | 1.86 | 0.97 | 0.48 | 2.84 | 1.24 | 1.20 | [148] |
| 1317 | C[S](C)=O | C1COCCO1 | 0.74 | 0.71 | 0.51 | 1.70 | 0.50 | 1.00 | 2.29 | 0.78 | 0.49 | [61] |
| 1318 | C[S](C)=O | CCOCC | 1.95 | 1.67 | 1.68 | 3.21 | 2.56 | 1.58 | 5.55 | 2.33 | 2.48 | [148] |
| 1319 | C[S](C)=O | CC(C)=O | 0.29 | 0.60 | 0.60 | 0.64 | 0.46 | 0.17 | 2.55 | 0.58 | 0.71 | [148] |
| 1320 | C[S](C)=O | CCC(C)=O | 0.66 | 0.90 | 0.90 | 0.88 | 0.88 | 0.42 | 3.11 | 0.89 | 0.83 | [148 , 61] |
| 1321 | C[S](C)=O | ClCCl | -0.67 | -0.43 | -0.42 | -0.27 | -0.45 | 0.24 | 2.36 | -1.05 | -0.58 | [148] |
| 1322 | C[S](C)=O | ClC(Cl)Cl | -0.25 | -1.08 | -1.08 | -0.84 | -0.45 | 0.80 | | -1.83 | -0.78 | [148] |
| 1323 | CCCCOCCCC | CCCCCC | 0.10 | 0.08 | 0.10 | 0.07 | 0.05 | -0.03 | -0.16 | 0.10 | 0.07 | [149 , 149 , 149 , 150] |
| 1324 | CCCCOCCCC | C1CCCCC1 | 0.06 | 0.05 | 0.07 | 0.05 | -0.06 | -0.08 | -0.30 | 0.12 | 0.09 | [57] |
| 1325 | CCCCOCCCC | CCCCCCCC | 0.14 | 0.15 | 0.15 | 0.10 | 0.17 | 0.09 | -0.17 | 0.19 | 0.08 | [149 , 149] |
| 1326 | CCCCOCCCC | CCC#CCC | -0.02 | -0.13 | -0.09 | -0.08 | | | | | 0.06 | [151] |
| 1327 | CCCOCCC | C1CCCCC1 | 0.13 | 0.18 | 0.15 | 0.13 | | 0.00 | -0.24 | 0.22 | 0.26 | [57] |
| 1328 | CCCS(=O)CCC | C1CCCC1 | 1.12 | | | | | 0.84 | 1.81 | | 1.46 | [61] |
| 1329 | CCCS(=O)CCC | C1CCCCC1 | 1.35 | | | | | 1.18 | 1.65 | | 1.72 | [61] |
| 1330 | CCCS(=O)CCC | CC1CCCC1 | 1.35 | | | | | | | | 1.72 | [61] |
| 1331 | CCCS(=O)CCC | CCCCCCC | 1.85 | | | | | 1.91 | 2.84 | | 2.27 | [61] |
| 1332 | CCCS(=O)CCC | CC1CCCCC1 | 1.54 | | | | | 1.44 | 2.24 | | 1.89 | [61] |
| 1333 | CCCS(=O)CCC | CC(C)CC(C)(C)C | 1.85 | | | | | 2.42 | 3.94 | | 2.39 | [61] |
| 1334 | CCCNCCC | CCCCCCC | 0.39 | 0.26 | 0.26 | 0.35 | | -0.01 | -0.15 | | 0.21 | [137] |
| 1335 | CCCSSCCC | CCCCCCC | 0.48 | 0.63 | 0.62 | 0.23 | | | | | 0.46 | [134 , 133] |
| 1336 | CCCSCCC | C1CCCCC1 | 0.30 | 0.15 | 0.15 | 0.19 | | | | | 0.37 | [134 , 133] |
| 1337 | CCCSCCC | CCCCCCC | 0.48 | 0.22 | 0.22 | 0.26 | | | | | 0.38 | [134 , 133] |
| 1338 | CCO | CCOC(=O)C | 0.57 | 1.20 | 1.12 | 1.02 | 1.15 | 0.56 | 1.13 | 1.26 | 1.28 | [61 , 123] |
| 1339 | CCO | C1COCCO1 | 0.31 | 0.97 | 0.98 | 1.49 | 0.28 | 1.09 | 0.60 | 1.08 | 1.13 | [61] |
| 1340 | CCO | CC(C)=O | 0.25 | 0.87 | 0.81 | 0.90 | 0.88 | 0.55 | 0.72 | 1.05 | 0.85 | [61] |
| 1341 | CCO | CCC(C)=O | 0.23 | 0.94 | 0.84 | 0.95 | 0.96 | 1.00 | 1.03 | 0.97 | 0.90 | [61] |
| 1342 | CCO | ClCCl | 0.34 | 0.96 | 0.88 | 0.77 | 0.69 | 0.63 | 0.62 | 1.18 | 0.92 | [61 , 123] |
| 1343 | CCO | ClC(Cl)Cl | 0.46 | 0.70 | 0.49 | 0.56 | 0.41 | 1.02 | | 1.05 | 0.54 | [61 , 123] |
| 1344 | CCO | ClC(Cl)(Cl)Cl | 2.05 | 1.58 | 1.42 | 1.60 | 1.89 | 2.53 | 1.48 | 1.85 | 1.64 | [61 , 123] |
| 1345 | CCO | CCBr | 1.15 | 1.27 | 1.17 | 1.39 | 1.42 | 1.18 | | | 1.41 | [61] |
| 1346 | CCO | CCI | 1.35 | 1.67 | 1.47 | 1.76 | 1.82 | | | | 1.79 | [61] |
| 1347 | CCO | CCN(CC)CC | 0.44 | 0.94 | 0.78 | 0.60 | 0.19 | 3.52 | 1.52 | 0.90 | 0.23 | [61] |
| 1348 | CCOc1ccccc1 | CCCCC | 0.71 | 0.70 | 0.62 | 0.71 | | | | | 0.90 | [61] |
| 1349 | CCOc1ccccc1 | CCCCCC | 0.81 | 0.82 | 0.72 | 0.76 | | | | | 0.98 | [61] |
| 1350 | CCOc1ccccc1 | C1CCCCC1 | 0.63 | 0.60 | 0.60 | 0.64 | | | | | 0.75 | [61] |
| 1351 | CCOc1ccccc1 | CCCC(C)C | 0.78 | 0.82 | 0.72 | 0.76 | | | | | 1.03 | [61] |
| 1352 | CCOc1ccccc1 | CCCCCCC | 0.90 | 0.92 | 0.83 | 0.81 | | | | | 1.08 | [61] |
| 1353 | CCOc1ccccc1 | CC(C)CC(C)C | 0.85 | 0.91 | 0.82 | 0.81 | | | | | 1.17 | [61] |
| 1354 | CCOc1ccccc1 | CCCCCCCC | 0.98 | 1.00 | 0.92 | 0.85 | | | | | 1.18 | [61 , 61] |
| 1355 | CCOc1ccccc1 | CC(C)C(C)C(C)C | 0.85 | 0.99 | 0.92 | 0.85 | | | | | 1.14 | [61] |
| 1356 | CCOc1ccccc1 | CCC1CCCCC1 | 0.79 | 0.82 | 0.81 | 0.73 | | | | | 0.96 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1357 | CCOc1ccccc1 | CCCCCCCCC | 1.06 | 1.07 | 1.01 | 0.90 | | | | | 1.36 | [61] |
| 1358 | CCOc1ccccc1 | CCC(C)CCC(C)C | 1.00 | 1.06 | 1.01 | 0.90 | | | | | 1.21 | [61] |
| 1359 | CCOc1ccccc1 | Cc1ccccc1 | 0.01 | 0.01 | 0.02 | -0.04 | | | | | 0.02 | [61] |
| 1360 | CCOc1ccccc1 | CCO | 2.53 | 1.68 | 1.37 | 1.72 | | | | | 2.29 | [61] |
| 1361 | CCOc1ccccc1 | C1COCCO1 | 0.01 | 0.66 | 0.10 | -0.16 | | | | | 0.10 | [61] |
| 1362 | CCOc1ccccc1 | CCC(C)=O | 0.17 | 0.18 | 0.10 | 0.17 | | | | | 0.17 | [61] |
| 1363 | CCOC(=O)C | CCCCC | 1.12 | 1.06 | 1.05 | 1.04 | 0.92 | 0.45 | 0.51 | 1.09 | 1.11 | [54 , 61 , 61] |
| 1364 | CCOC(=O)C | CCCCCC | 1.27 | 1.21 | 1.21 | 1.19 | 1.07 | 0.52 | 0.41 | 1.22 | 1.28 | [54 , 61 , 61 , 119] |
| 1365 | CCOC(=O)C | C1CCCCC1 | 1.09 | 1.12 | 1.03 | 1.21 | 0.85 | 0.36 | -0.04 | 1.24 | 1.19 | [54 , 61] |
| 1366 | CCOC(=O)C | CCCC(C)C | 1.22 | 1.21 | 1.21 | 1.19 | 1.09 | | | 1.22 | 1.24 | [54 , 61 , 61] |
| 1367 | CCOC(=O)C | CCCCCCC | 1.41 | 1.34 | 1.36 | 1.34 | 1.21 | 0.60 | 0.32 | 1.35 | 1.37 | [54 , 61 , 61] |
| 1368 | CCOC(=O)C | CC(C)CC(C)C | 1.30 | 1.34 | 1.36 | 1.34 | 1.21 | | | 1.34 | 1.34 | [54 , 61 , 61] |
| 1369 | CCOC(=O)C | CCCCCCCC | 1.55 | 1.45 | 1.50 | 1.49 | 1.40 | 0.69 | 0.29 | 1.47 | 1.56 | [54 , 61 , 61 , 61] |
| 1370 | CCOC(=O)C | CC(C)C(C)C(C)C | 1.35 | 1.45 | 1.50 | 1.49 | 1.09 | | | | 1.40 | [54 , 61 , 61] |
| 1371 | CCOC(=O)C | CC(C)CCC(C)C | 1.46 | 1.45 | 1.50 | 1.49 | | | | | 1.47 | [54] |
| 1372 | CCOC(=O)C | CCC1CCCCC1 | 1.34 | 1.40 | 1.33 | 1.46 | | | | 1.50 | 2.99 | [54 , 61 , 61] |
| 1373 | CCOC(=O)C | CCCCCCCCC | 1.68 | 1.56 | 1.64 | 1.64 | 1.67 | 0.78 | 0.25 | 1.60 | 1.70 | [54 , 61 , 61] |
| 1374 | CCOC(=O)C | CCC(C)CCC(C)C | 1.57 | 1.56 | 1.64 | 1.64 | | | | | 1.37 | [61] |
| 1375 | CCOC(=O)C | Cc1ccccc1 | 0.23 | 0.24 | 0.02 | 0.35 | 0.28 | 0.22 | -0.16 | 0.25 | 0.29 | [61 , 152 , 152] |
| 1376 | CCOC(=O)C | CCCC=C | 0.59 | 0.65 | 0.64 | 0.62 | 0.78 | 0.10 | 0.50 | 0.77 | 0.71 | [61] |
| 1377 | CCOC(=O)C | CC(C)C=C | 0.58 | 0.65 | 0.64 | 0.62 | | | | | 0.71 | [61] |
| 1378 | CCOC(=O)C | CC(=C)C=C | 0.26 | 0.41 | 0.41 | 0.63 | 0.54 | | | | 0.28 | [61] |
| 1379 | CCOC(=O)C | CCCCCC=C | 0.86 | 0.93 | 0.94 | 0.95 | 0.98 | 0.24 | 0.32 | | 1.23 | [61] |
| 1380 | CCOC(=O)C | CCO | 0.74 | 1.13 | 1.07 | 1.06 | 0.97 | 0.22 | 2.12 | 1.60 | 1.22 | [61] |
| 1381 | CCOC(=O)C | C1CCOC1 | 0.06 | 0.08 | 0.08 | 0.34 | -0.25 | -0.22 | -0.21 | 0.04 | 0.13 | [61] |
| 1382 | CCOC(=O)C | C1COCCO1 | -0.02 | 0.04 | -0.12 | 0.01 | 0.02 | 0.05 | -0.09 | 0.17 | 0.08 | [61] |
| 1383 | CCOC(=O)C | CC(C)=O | 0.13 | 0.26 | 0.29 | 0.10 | 0.49 | -0.16 | -0.21 | 0.05 | 0.12 | [61] |
| 1384 | CCOC(=O)C | CCC(C)=O | 0.04 | 0.25 | 0.25 | 0.10 | 0.44 | -0.12 | -0.21 | -0.02 | 0.14 | [61] |
| 1385 | CCOC(=O)C | CCCCl | 0.01 | 0.10 | 0.10 | 0.07 | 0.22 | | | | 0.10 | [61] |
| 1386 | CCOC(=O)C | CC(C)(C)Cl | 0.05 | 0.54 | 0.54 | 0.51 | 0.43 | | | | 0.19 | [61] |
| 1387 | CCOC(=O)C | ClCCl | -0.99 | -0.78 | -0.73 | -0.63 | -0.67 | -0.22 | -0.22 | -0.65 | -0.69 | [61] |
| 1388 | CCOC(=O)C | ClC(Cl)Cl | -0.94 | -0.73 | -0.76 | -0.92 | -0.89 | -0.14 | | -1.17 | -0.92 | [61] |
| 1389 | CCOC(=O)C | ClC(Cl)(Cl)Cl | 0.81 | 0.24 | 0.22 | 0.23 | 0.27 | 0.32 | -0.17 | 0.31 | 0.26 | [61] |
| 1390 | CCOC(=O)C | CCBr | -0.27 | 0.06 | 0.09 | 0.11 | 0.20 | -0.12 | | | 0.04 | [61] |
| 1391 | CCOC(=O)C | CCC#N | 0.19 | 0.36 | 0.38 | 0.24 | 0.82 | 0.07 | 0.08 | 0.19 | 0.39 | [61] |
| 1392 | CCOC(=O)C | CCI | -0.22 | 0.43 | 0.41 | 0.43 | 0.69 | | | | 0.43 | [61] |
| 1393 | CCOC(=O)C | CCN(CC)CC | 0.25 | 0.94 | 0.96 | 0.83 | 0.88 | 0.54 | -0.09 | 0.85 | 0.74 | [61] |
| 1394 | CCOC(=O)C | C(=S)=S | 0.71 | 0.92 | 0.94 | 0.92 | | 0.24 | -0.20 | | 0.96 | [61] |
| 1395 | CCBr | CCCCC | 1.02 | 0.59 | 0.65 | 0.36 | | | 0.70 | | 0.59 | [61] |
| 1396 | CCBr | C1CCCCC1 | 0.98 | 0.62 | 0.62 | 0.70 | | | 0.12 | | 0.56 | [61] |
| 1397 | CCBr | CCCCCCC | 1.26 | 0.60 | 0.78 | 0.36 | | | 0.49 | | 0.66 | [61] |
| 1398 | CCBr | CCCCCCCC | 1.38 | 0.58 | 0.84 | 0.36 | | | 0.46 | | 0.77 | [61 , 61] |
| 1399 | CCBr | CC(C)C(C)C(C)C | 1.19 | 0.58 | 0.84 | 0.36 | | | | | 0.66 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1400 | CCBr | CCCCCCCCC | 1.47 | 0.54 | 0.89 | 0.36 | | | 0.41 | | 0.89 | [61] |
| 1401 | CCBr | CCC(C)CCC(C)C | 1.39 | 0.54 | 0.89 | 0.36 | | | | | 0.62 | [61] |
| 1402 | CCBr | Cc1ccccc1 | -0.24 | 0.54 | 0.43 | 0.02 | | | -0.06 | | 0.07 | [61] |
| 1403 | CCBr | C1COCCO1 | -0.21 | 0.34 | 0.16 | 0.25 | | | -0.15 | | 0.28 | [61] |
| 1404 | CCBr | CCC(C)=O | -0.15 | 0.11 | 0.14 | 0.11 | | | -0.15 | | 0.03 | [61] |
| 1405 | CCCCOCC | C1CCCCC1 | 0.16 | 0.18 | 0.15 | 0.13 | | | | | 0.36 | [57] |
| 1406 | CCCC(=O)OCC | CCCCC | 0.63 | 0.41 | 0.43 | 0.50 | | | | | 0.55 | [54] |
| 1407 | CCCC(=O)OCC | CCCCCC | 0.73 | 0.50 | 0.50 | 0.59 | | | | | 0.68 | [54] |
| 1408 | CCCC(=O)OCC | C1CCCCC1 | 0.61 | 0.46 | 0.42 | 0.64 | | | | | 0.62 | [54] |
| 1409 | CCCC(=O)OCC | CCCC(C)C | 0.70 | 0.50 | 0.50 | 0.59 | | | | | 0.66 | [54] |
| 1410 | CCCC(=O)OCC | CCCCCCC | 0.82 | 0.58 | 0.57 | 0.67 | | | | | 0.69 | [54] |
| 1411 | CCCC(=O)OCC | CC(C)CC(C)C | 0.75 | 0.58 | 0.57 | 0.67 | | | | | 0.73 | [54] |
| 1412 | CCCC(=O)OCC | CCCCCCCC | 0.90 | 0.64 | 0.64 | 0.75 | | | | | 0.88 | [54] |
| 1413 | CCCC(=O)OCC | CC(C)C(C)C(C)C | 0.77 | 0.64 | 0.64 | 0.75 | | | | | 0.77 | [54] |
| 1414 | CCCC(=O)OCC | CC(C)CCC(C)C | 0.85 | 0.64 | 0.64 | 0.75 | | | | | 0.81 | [54] |
| 1415 | CCCC(=O)OCC | CCC1CCCCC1 | 0.77 | 0.63 | 0.56 | 0.78 | | | | | 0.79 | [54] |
| 1416 | CCCC(=O)OCC | CCCCCCCCC | 0.98 | 0.68 | 0.69 | 0.83 | | | | | 0.98 | [54] |
| 1417 | CCc1ccccc1 | CCCCCCC | 0.53 | 0.41 | 0.29 | 0.36 | 0.60 | 0.09 | 0.21 | 0.58 | 0.51 | [108] |
| 1418 | C1COC(=O)O1 | CCCCCC | 4.58 | | | 3.60 | | 4.50 | 6.14 | | 4.50 | [47 , 73] |
| 1419 | C1COC(=O)O1 | c1ccccc1 | 1.78 | | | 0.96 | | 2.47 | 3.48 | | 1.02 | [47 , 73] |
| 1420 | C(CO)O | CCCCCC | 4.93 | 5.49 | 5.57 | 5.25 | 6.27 | 6.39 | 5.00 | | 6.11 | [73 , 154 , 153 , 153 , 59 , 47] |
| 1421 | C(CO)O | c1ccccc1 | 2.63 | 3.25 | 2.98 | 3.32 | 3.66 | 3.69 | 2.81 | | 3.48 | [73 , 154 , 59 , 155] |
| 1422 | C(CO)O | CCCCC | 4.33 | 4.79 | 4.82 | 4.63 | 5.71 | 5.66 | 5.26 | | 5.52 | [153 , 153 , 153] |
| 1423 | C(CO)O | C1CCCCC1 | 4.28 | 4.80 | 4.69 | -0.14 | 5.85 | 5.07 | 3.78 | | 5.58 | [154 , 155] |
| 1424 | C(CO)O | CCCCCCC | 5.52 | 6.18 | 6.30 | 5.88 | 6.81 | 7.13 | 4.74 | | 6.88 | [154 , 153 , 153 , 155] |
| 1425 | C(CO)O | CCCCCCCC | 6.11 | 6.84 | 7.04 | 6.51 | 7.41 | 7.89 | 4.62 | | 7.48 | [154 , 153 , 153 , 155] |
| 1426 | C(CO)O | CCCCCCCCC | 6.69 | 7.49 | 7.77 | 7.14 | 8.09 | 8.65 | 4.50 | | 7.72 | [154 , 155] |
| 1427 | C(CO)O | Cc1ccccc1 | 3.07 | 4.21 | 3.94 | 4.06 | 4.16 | 4.25 | 3.02 | | 4.16 | [154 , 155] |
| 1428 | C(CO)O | CC1CCCCC1 | 4.77 | 5.50 | 5.43 | 0.93 | 6.30 | 5.73 | 4.26 | | 6.30 | [155] |
| 1429 | C(CO)O | CC(C)CC(C)(C)C | 5.47 | 6.91 | 7.14 | 6.50 | 6.83 | 8.26 | 5.57 | | 7.05 | [155] |
| 1430 | C(CO)O | CCC1CCCCC1 | 5.32 | 6.18 | 6.17 | 1.57 | | | | | 6.65 | [155] |
| 1431 | C(CO)O | Cc1cccc(C)c1 | 3.44 | 5.10 | 4.86 | 4.82 | 4.61 | 4.62 | 3.07 | | 4.82 | [155] |
| 1432 | C(CO)O | Cc1ccc(C)cc1 | 3.53 | 5.10 | 4.86 | 4.82 | 4.56 | 4.58 | 3.17 | | 4.81 | [155] |
| 1433 | C(CO)O | Cc1ccccc1C | 3.49 | 5.10 | 4.86 | 4.82 | 4.55 | 4.51 | 3.07 | | 4.67 | [155] |
| 1434 | C(CO)O | CCc1ccccc1 | 3.45 | 4.82 | 4.60 | 4.84 | 4.66 | 5.24 | 3.19 | | 4.72 | [155] |
| 1435 | C(CO)O | CCCc1ccccc1 | 4.04 | 5.47 | 5.30 | 5.48 | 5.15 | | | | 5.31 | [155] |
| 1436 | C(CO)O | CC(C)c1ccccc1 | 3.85 | 5.42 | 5.24 | 5.22 | 5.02 | 6.03 | 3.04 | | 5.21 | [155] |
| 1437 | C(CO)O | CCCCC=C | 4.12 | 3.38 | 3.42 | 3.24 | 5.49 | 6.00 | 5.10 | | 5.67 | [155] |
| 1438 | C(CO)O | CCC\C=C/C | 4.07 | 3.85 | 3.89 | 3.61 | | | | | 5.59 | [155] |
| 1439 | C(CO)O | C1CCC=CC1 | 3.56 | 3.17 | 3.03 | -0.29 | 5.09 | 3.23 | 3.13 | | 4.85 | [155] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1440 | C(CO)O | CCCCCC=C | 4.67 | 4.06 | 4.15 | 3.88 | 5.95 | 5.59 | 4.76 | | 6.23 | [155] |
| 1441 | C(CO)O | CCCCCCC=C | 5.34 | 4.72 | 4.88 | 4.51 | 6.56 | 6.07 | 4.60 | | 6.82 | [155] |
| 1442 | C(CO)O | CC(=C)CC(C)(C)C | 4.73 | 5.22 | 5.46 | 4.89 | | | | | 6.51 | [155] |
| 1443 | NCCN | CCCCCC | 3.79 | 2.30 | 2.36 | 3.48 | | 2.91 | 2.79 | | 4.38 | [47 , 73] |
| 1444 | NCCN | c1ccccc1 | 1.53 | 0.84 | 0.64 | 1.18 | | 1.56 | 1.08 | | 1.86 | [47 , 73] |
| 1445 | CCOC(C)(C)C | CCCCCC | 0.25 | 0.18 | 0.17 | 0.12 | | | | | 0.16 | [132] |
| 1446 | CCOC(C)(C)C | C1CCCCC1 | 0.22 | 0.21 | 0.14 | 0.13 | | | | | 0.18 | [132] |
| 1447 | CCOC(C)(C)C | CCCCCCC | 0.28 | 0.21 | 0.20 | 0.13 | | | | | 0.19 | [132] |
| 1448 | Fc1ccccc1 | CCCCC | 0.65 | 0.58 | 0.43 | 0.78 | 0.63 | 0.63 | 0.90 | | 0.65 | [61] |
| 1449 | Fc1ccccc1 | CCCCCC | 0.72 | 0.60 | 0.48 | 0.74 | 0.70 | 0.66 | 0.77 | | 0.70 | [61] |
| 1450 | Fc1ccccc1 | C1CCCCC1 | 0.58 | 0.43 | 0.41 | 0.81 | 0.59 | 0.20 | 0.17 | | 0.65 | [61] |
| 1451 | Fc1ccccc1 | CCCC(C)C | 0.69 | 0.60 | 0.48 | 0.74 | 0.74 | | | | 0.72 | [61] |
| 1452 | Fc1ccccc1 | CCCCCCC | 0.78 | 0.61 | 0.52 | 0.70 | 0.76 | 0.67 | 0.65 | | 0.77 | [61] |
| 1453 | Fc1ccccc1 | CC(C)CC(C)C | 0.73 | 0.60 | 0.52 | 0.70 | 0.82 | | | | 0.77 | [61] |
| 1454 | Fc1ccccc1 | CCCCCCCC | 0.84 | 0.60 | 0.56 | 0.66 | 0.87 | 0.72 | 0.60 | | 0.87 | [61] |
| 1455 | Fc1ccccc1 | CCC1CCCCC1 | 0.70 | 0.46 | 0.50 | 0.72 | | | | | 0.82 | [61] |
| 1456 | Fc1ccccc1 | CCCCCCCCC | 0.88 | 0.58 | 0.59 | 0.62 | 1.05 | 0.76 | 0.55 | | 1.01 | [61] |
| 1457 | O=Cc1occc1 | CCCCC | 2.46 | 2.09 | 2.02 | 3.01 | | 2.07 | 2.23 | | 3.04 | [156 , 156 , 157] |
| 1458 | O=Cc1occc1 | C1CCCC1 | 2.06 | 1.65 | 1.65 | 2.22 | | 1.27 | 1.21 | | 2.49 | [156 , 156 , 157] |
| 1459 | O=Cc1occc1 | CCCCCC | 2.80 | 2.36 | 2.33 | 3.24 | | 2.29 | 2.03 | | 3.29 | [156 , 156 , 73 , 157] |
| 1460 | O=Cc1occc1 | C1CCCCC1 | 2.35 | 1.95 | 1.96 | 2.57 | | 1.56 | 1.11 | | 2.70 | [156 , 156 , 157] |
| 1461 | O=Cc1occc1 | CCCCCCC | 3.13 | 2.61 | 2.62 | 3.47 | | 2.50 | 1.84 | | 3.48 | [156 , 156 , 157] |
| 1462 | O=Cc1occc1 | c1ccccc1 | 0.80 | 0.69 | 0.68 | 0.85 | | 1.07 | 0.47 | | 0.93 | [156 , 156 , 73 , 157] |
| 1463 | O=Cc1occc1 | Cc1ccccc1 | 1.05 | 1.17 | 1.17 | 0.91 | | 1.11 | 0.61 | | 1.28 | [156 , 156] |
| 1464 | O=Cc1occc1 | Cc1ccccc1C | 1.20 | 1.57 | 1.61 | 0.98 | | 1.34 | 0.66 | | 1.37 | [156 , 156] |
| 1465 | O=Cc1occc1 | CCc1ccccc1 | 1.30 | 1.37 | 1.41 | 1.42 | | 1.52 | 0.73 | | 1.54 | [156 , 156] |
| 1466 | O=Cc1occc1 | C1CCCCCC1 | 2.56 | 2.22 | 2.27 | 2.90 | | | | | 2.74 | [157] |
| 1467 | O=Cc1occc1 | CCCCC=C | 2.03 | 2.42 | 2.38 | 2.41 | | 2.01 | 2.12 | | 2.71 | [157] |
| 1468 | O=Cc1occc1 | CCCCCC=C | 2.33 | 2.67 | 2.67 | 2.65 | | 2.03 | 1.86 | | 2.88 | [157] |
| 1469 | O=Cc1occc1 | CCCCC#C | 1.04 | 0.67 | 0.68 | 1.64 | | | | | 1.40 | [157] |
| 1470 | O=Cc1occc1 | CCCCCC#C | 1.34 | 0.82 | 0.88 | 1.84 | | | | | 1.63 | [157] |
| 1471 | C1=COC(=C1)CO | CCCCC | 2.31 | | | | | 2.09 | 4.19 | | 3.21 | [158] |
| 1472 | C1=COC(=C1)CO | C1CCCC1 | 1.95 | | | | | 1.18 | 2.73 | | 2.48 | [158] |
| 1473 | C1=COC(=C1)CO | CCCCCC | 2.62 | | | | | 2.35 | 3.91 | | 3.43 | [158] |
| 1474 | C1=COC(=C1)CO | C1CCCCC1 | 2.21 | | | | | 1.70 | 2.57 | | 2.73 | [158] |
| 1475 | C1=COC(=C1)CO | CCCCCCC | 2.92 | | | | | 2.60 | 3.63 | | 3.62 | [158] |
| 1476 | C1=COC(=C1)CO | C1CCCCCC1 | 2.41 | | | | | | | | 2.87 | [158] |
| 1477 | C1=COC(=C1)CO | c1ccccc1 | 1.00 | | | | | 1.07 | 1.58 | | 1.15 | [158] |
| 1478 | C1=COC(=C1)CO | CCCCC=C | 1.99 | | | | | 2.17 | 4.02 | | 2.81 | [158] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1479 | C1=COC(=C1)CO | CCCCCC=C | 2.25 | | | | | 1.79 | 3.65 | | 3.01 | [158] |
| 1480 | C1=COC(=C1)CO | CCCCC#C | 1.26 | | | | | | | | 1.80 | [158] |
| 1481 | C1=COC(=C1)CO | CCCCCC#C | 1.53 | | | | | | | | 1.91 | [158] |
| 1482 | O=C1CCCO1 | CCCCC | 2.82 | 2.12 | 2.09 | 1.90 | | 2.76 | 3.82 | | 3.14 | [54] |
| 1483 | O=C1CCCO1 | CCCCCC | 3.23 | 2.42 | 2.41 | 2.09 | | 3.05 | 3.56 | | 3.56 | [54] |
| 1484 | O=C1CCCO1 | C1CCCCC1 | 2.76 | 2.20 | 2.04 | 1.94 | | 2.15 | 2.37 | | 3.04 | [54] |
| 1485 | O=C1CCCO1 | CCCC(C)C | 3.12 | 2.42 | 2.41 | 2.09 | | | | | 3.47 | [54] |
| 1486 | O=C1CCCO1 | CCCCCCC | 3.63 | 2.71 | 2.72 | 2.28 | | 3.34 | 3.31 | | 3.94 | [54] |
| 1487 | O=C1CCCO1 | CC(C)CC(C)C | 3.40 | 2.71 | 2.71 | 2.28 | | | | | 3.82 | [54] |
| 1488 | O=C1CCCO1 | CCCCCCCC | 4.02 | 2.98 | 3.02 | 2.46 | | 3.66 | 3.20 | | 4.33 | [54] |
| 1489 | O=C1CCCO1 | CC(C)C(C)C(C)C | 3.59 | 2.98 | 3.02 | 2.46 | | | | | 3.97 | [54] |
| 1490 | O=C1CCCO1 | CC(C)CCC(C)C | 3.83 | 2.98 | 3.02 | 2.46 | | | | | 4.20 | [54] |
| 1491 | O=C1CCCO1 | CCC1CCCCC1 | 3.48 | 2.79 | 2.66 | 2.21 | | | | | 3.74 | [54] |
| 1492 | O=C1CCCO1 | CCCCCCCCC | 4.41 | 3.24 | 3.32 | 2.64 | | 3.98 | 3.08 | | 4.67 | [54] |
| 1493 | C1COS(=O)O1 | C1CCCC1 | 2.46 | | | | | | | | 2.72 | [84] |
| 1494 | C1COS(=O)O1 | CCCCCC | 3.33 | | | | | | | | 3.61 | [84] |
| 1495 | C1COS(=O)O1 | C1CCCCC1 | 2.81 | | | | | | | | 3.08 | [84] |
| 1496 | C1COS(=O)O1 | CC1CCCC1 | 2.85 | | | | | | | | 3.10 | [84] |
| 1497 | C1COS(=O)O1 | CCCCCCC | 3.71 | | | | | | | | 3.82 | [84] |
| 1498 | C1COS(=O)O1 | CC1CCCCC1 | 3.15 | | | | | | | | 3.35 | [84] |
| 1499 | C1COS(=O)O1 | CC(C)CC(C)(C)C | 3.71 | | | | | | | | 3.90 | [84] |
| 1500 | C1COS(=O)O1 | c1ccccc1 | 0.83 | | | | | | | | 0.99 | [84] |
| 1501 | C1COS(=O)O1 | Cc1ccccc1 | 1.22 | | | | | | | | 1.39 | [84] |
| 1502 | CCCCCCC#N | CCCCCC | 1.14 | 0.85 | 0.85 | 1.16 | | | | | 1.10 | [47 , 98] |
| 1503 | CCCCCCC#N | C1CCCCC1 | 0.94 | 0.71 | 0.71 | 0.97 | | | | | 0.95 | [47 , 98] |
| 1504 | CCCCCCC#N | c1ccccc1 | 0.07 | -0.02 | -0.05 | 0.03 | | | | | -0.11 | [47] |
| 1505 | CCCCCCC#N | CC=C(C)C | 0.52 | 0.51 | 0.52 | 0.74 | | | | | 0.63 | [47] |
| 1506 | CCCCCCC#N | CC(=C)C=C | 0.29 | 0.17 | 0.23 | 0.22 | | | | | 0.26 | [47] |
| 1507 | NCCCCCCCN | CCCCCCC | 1.46 | 1.06 | 1.07 | 1.63 | | | | | 0.89 | [137] |
| 1508 | CCCCCCCN | CCCCCCC | 0.57 | 0.43 | 0.43 | 0.60 | | 0.36 | 0.07 | | 0.56 | [137] |
| 1509 | OC(F)(C(F)F)C(F)(F)F | CCCCC | 2.65 | 2.47 | 2.34 | 3.59 | | 1.68 | 2.95 | | 1.46 | [54] |
| 1510 | OC(F)(C(F)F)C(F)(F)F | CCCCCC | 3.11 | 2.91 | 2.72 | 3.98 | | 1.89 | 2.69 | | 3.18 | [54] |
| 1511 | OC(F)(C(F)F)C(F)(F)F | C1CCCCC1 | 2.79 | 2.65 | 2.28 | 3.63 | | 1.32 | 1.48 | | 3.22 | [54] |
| 1512 | OC(F)(C(F)F)C(F)(F)F | CCCC(C)C | 2.99 | 2.91 | 2.72 | 3.98 | | | | | 2.89 | [54] |
| 1513 | OC(F)(C(F)F)C(F)(F)F | CCCCCCC | 3.54 | 3.33 | 3.09 | 4.37 | | 2.10 | 2.44 | | 3.67 | [54] |
| 1514 | OC(F)(C(F)F)C(F)(F)F | CC(C)CC(C)C | 3.28 | 3.33 | 3.09 | 4.37 | | | | | 3.21 | [54] |
| 1515 | OC(F)(C(F)F)C(F)(F)F | CCCCCCCC | 3.98 | 3.73 | 3.46 | 4.75 | | 2.33 | 2.33 | | 4.17 | [54] |
| 1516 | OC(F)(C(F)F)C(F)(F)F | CC(C)C(C)C(C)C | 3.53 | 3.73 | 3.45 | 4.75 | | | | | 3.63 | [54] |
| 1517 | OC(F)(C(F)F)C(F)(F)F | CC(C)CCC(C)C | 3.73 | 3.73 | 3.45 | 4.75 | | | | | 3.72 | [54] |
| 1518 | OC(F)(C(F)F)C(F)(F)F | CCC1CCCCC1 | 3.57 | 3.51 | 3.03 | 4.21 | | | | | 4.04 | [54] |
| 1519 | OC(F)(C(F)F)C(F)(F)F | CCCCCCCCC | 4.41 | 4.12 | 3.82 | 5.13 | | 2.56 | 2.21 | | 4.64 | [54] |
| 1520 | Fc1c(F)c(F)c(F)c(F)c1F | CCCCCCCCCCCCCC | 2.50 | 2.33 | 2.47 | 1.75 | | -0.03 | -0.04 | | 2.05 | [159] |
| 1521 | CN(C)[P](=O)(N(C)C)N(C)C | CCCCC | 0.96 | | | | | 1.53 | 4.99 | | 1.36 | [54 , 47] |
| 1522 | CN(C)[P](=O)(N(C)C)N(C)C | CCC(C)C | 0.91 | | | | | 1.77 | 6.02 | | 1.70 | [47] |
| 1523 | CN(C)[P](=O)(N(C)C)N(C)C | CCCCCC | 1.16 | | | | | 1.73 | 4.56 | | 1.58 | [54 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1524 | CN(C)[P](=O)(N(C)C)N(C)C | C1CCCCC1 | 0.94 | | | | | 1.02 | 2.53 | | 1.18 | [54 , 47] |
| 1525 | CN(C)[P](=O)(N(C)C)N(C)C | CCCC(C)C | 1.11 | | | | | | | | 1.35 | [54] |
| 1526 | CN(C)[P](=O)(N(C)C)N(C)C | CCCCCCC | 1.34 | | | | | 1.91 | 4.14 | | 1.55 | [54] |
| 1527 | CN(C)[P](=O)(N(C)C)N(C)C | CC(C)CC(C)C | 1.24 | | | | | | | | 1.52 | [54] |
| 1528 | CN(C)[P](=O)(N(C)C)N(C)C | CCCCCCCC | 1.52 | | | | | 2.13 | 3.95 | | 1.72 | [54] |
| 1529 | CN(C)[P](=O)(N(C)C)N(C)C | CC(C)C(C)C(C)C | 1.33 | | | | | | | | 1.56 | [54] |
| 1530 | CN(C)[P](=O)(N(C)C)N(C)C | CC(C)CCC(C)C | 1.44 | | | | | | | | 1.69 | [54] |
| 1531 | CN(C)[P](=O)(N(C)C)N(C)C | CCC1CCCCC1 | 1.28 | | | | | | | | 1.38 | [54] |
| 1532 | CN(C)[P](=O)(N(C)C)N(C)C | CCCCCCCCC | 1.70 | | | | | 2.33 | 3.76 | | 1.89 | [54] |
| 1533 | CN(C)[P](=O)(N(C)C)N(C)C | c1ccccc1 | -0.20 | | | | | 0.44 | 1.12 | | -0.25 | [47] |
| 1534 | CN(C)[P](=O)(N(C)C)N(C)C | CC=C(C)C | 0.47 | | | | | 0.74 | 4.42 | | 1.02 | [47] |
| 1535 | CN(C)[P](=O)(N(C)C)N(C)C | CC(=C)C=C | 0.14 | | | | | | | | 0.38 | [47] |
| 1536 | CCCCCC#N | CCCCCC | 1.37 | 1.03 | 1.03 | 1.33 | | 0.70 | 0.48 | | 1.38 | [98 , 47] |
| 1537 | CCCCCC#N | C1CCCCC1 | 1.15 | 0.88 | 0.86 | 1.14 | | 0.55 | -0.07 | | 1.18 | [98 , 47] |
| 1538 | CCCCCC#N | c1ccccc1 | 0.16 | 0.08 | 0.01 | 0.11 | | 0.44 | -0.29 | | 0.04 | [47] |
| 1539 | CCCCCC#N | CC=C(C)C | 0.68 | 0.67 | 0.66 | 0.88 | | 0.17 | 0.41 | | 0.81 | [47] |
| 1540 | CCCCCC#N | CC(=C)C=C | 0.41 | 0.29 | 0.32 | 0.30 | | | | | 0.39 | [47] |
| 1541 | NCCCCCCN | C1CCCCC1 | 1.28 | 0.92 | 0.91 | 1.39 | | | | | 0.67 | [160] |
| 1542 | NCCCCCCN | CCCCCCC | 1.77 | 1.25 | 1.25 | 1.85 | | | | | 0.90 | [137] |
| 1543 | CCCCCCOC(=O)C | CCCCC | 0.43 | 0.19 | 0.24 | 0.33 | | 0.05 | 0.16 | | 0.39 | [54] |
| 1544 | CCCCCCOC(=O)C | CCCCCC | 0.51 | 0.29 | 0.31 | 0.39 | | 0.10 | 0.07 | | 0.52 | [54] |
| 1545 | CCCCCCOC(=O)C | C1CCCCC1 | 0.40 | 0.24 | 0.24 | 0.41 | | -0.03 | -0.31 | | 0.41 | [54] |
| 1546 | CCCCCCOC(=O)C | CCCC(C)C | 0.48 | 0.29 | 0.31 | 0.39 | | | | | 0.51 | [54] |
| 1547 | CCCCCCOC(=O)C | CCCCCCC | 0.58 | 0.36 | 0.37 | 0.45 | | 0.17 | -0.01 | | 0.60 | [54] |
| 1548 | CCCCCCOC(=O)C | CC(C)CC(C)C | 0.52 | 0.36 | 0.37 | 0.45 | | | | | 0.51 | [54] |
| 1549 | CCCCCCOC(=O)C | CCCCCCCC | 0.65 | 0.43 | 0.43 | 0.51 | | 0.23 | -0.02 | | 0.68 | [54] |
| 1550 | CCCCCCOC(=O)C | CC(C)C(C)C(C)C | 0.54 | 0.43 | 0.43 | 0.51 | | | | | 0.58 | [54] |
| 1551 | CCCCCCOC(=O)C | CC(C)CCC(C)C | 0.60 | 0.43 | 0.43 | 0.51 | | | | | 0.65 | [54] |
| 1552 | CCCCCCOC(=O)C | CCC1CCCCC1 | 0.54 | 0.41 | 0.36 | 0.51 | | | | | 0.55 | [54] |
| 1553 | CCCCCCOC(=O)C | CCCCCCCCC | 0.71 | 0.48 | 0.47 | 0.57 | | 0.29 | -0.04 | | 0.77 | [54] |
| 1554 | CCCCCCN | CCCCCCC | 0.68 | 0.52 | 0.52 | 0.68 | | 0.43 | 0.08 | | 0.77 | [137] |
| 1555 | CC(O)C#N | CCCCCC | 5.51 | 3.55 | 3.47 | 5.79 | | | | | 4.38 | [47 , 47] |
| 1556 | CC(O)C#N | c1ccccc1 | 2.56 | 1.67 | 1.31 | 2.44 | | | | | 2.05 | [73 , 73] |
| 1557 | N#CCCNCCC#N | CCCCCC | 4.48 | 2.99 | 2.99 | 4.50 | | | | | 4.56 | [47 , 47] |
| 1558 | N#CCCNCCC#N | c1ccccc1 | 1.56 | 0.67 | 0.66 | 1.18 | | | | | 1.16 | [73 , 73] |
| 1559 | C1C=Cc2ccccc12 | CCCCC | 0.80 | 0.92 | 0.49 | 1.31 | | 0.91 | 1.70 | | 1.10 | [61 , 47] |
| 1560 | C1C=Cc2ccccc12 | CCC(C)C | 0.78 | 0.91 | 0.49 | 1.31 | | 1.14 | 2.21 | | 1.17 | [61 , 47] |
| 1561 | C1C=Cc2ccccc12 | CCCCCC | 0.90 | 1.03 | 0.57 | 1.36 | | 0.99 | 1.50 | | 1.06 | [61 , 47] |
| 1562 | C1C=Cc2ccccc12 | C1CCCCC1 | 0.68 | 0.67 | 0.48 | 1.00 | | 0.44 | 0.57 | | 0.78 | [61 , 47] |
| 1563 | C1C=Cc2ccccc12 | c1ccccc1 | -0.05 | 0.00 | -0.02 | 0.05 | | 0.04 | 0.00 | | 0.01 | [61 , 47] |
| 1564 | C1C=Cc2ccccc12 | CC=C(C)C | 0.41 | 0.91 | 0.37 | 0.96 | | 0.46 | 1.42 | | 0.68 | [47] |
| 1565 | C1C=Cc2ccccc12 | CC(=C)C=C | 0.14 | 0.57 | 0.27 | 0.38 | | | | | 0.44 | [61 , 47] |
| 1566 | CI | CCCCC | 1.31 | 1.09 | 1.20 | 1.17 | | | | 1.73 | 3.29 | [61] |
| 1567 | CI | CCCCCC | 1.48 | 1.15 | 1.35 | 1.21 | | | | 1.68 | 3.61 | [61] |
| 1568 | CI | C1CCCCC1 | 1.24 | 1.04 | 1.15 | -1.83 | | | | 0.92 | 2.60 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1569 | CI | CCCC(C)C | 1.44 | 1.14 | 1.35 | 1.21 | | | | 1.93 | 3.71 | [61] |
| 1570 | CI | CCCCCCC | 1.61 | 1.18 | 1.50 | 1.24 | | | | 1.68 | 3.94 | [61] |
| 1571 | CI | CC(C)CC(C)C | 1.52 | 1.18 | 1.49 | 1.24 | | | | 2.17 | 4.14 | [61] |
| 1572 | CI | CCCCCCCC | 1.76 | 1.20 | 1.63 | 1.28 | | | | 1.69 | 4.13 | [61 , 61] |
| 1573 | CI | CC(C)C(C)C(C)C | 1.52 | 1.20 | 1.63 | 1.28 | | | | | 4.07 | [61] |
| 1574 | CI | CCC1CCCCC1 | 1.48 | 1.13 | 1.44 | -1.35 | | | | 1.21 | 3.30 | [61] |
| 1575 | CI | CCCCCCCCC | 1.89 | 1.21 | 1.77 | 1.32 | | | | 1.68 | 4.58 | [61] |
| 1576 | CI | CCC(C)CCC(C)C | 1.78 | 1.21 | 1.76 | 1.32 | | | | | 4.36 | [61] |
| 1577 | CI | Cc1ccccc1 | -0.31 | 0.20 | 0.22 | 0.27 | | | | 0.27 | 1.35 | [61] |
| 1578 | CC(C)N | CCCCCCC | 1.41 | 0.53 | 0.62 | 0.82 | | 0.48 | -0.01 | | 0.83 | [137] |
| 1579 | Cc1ccccc(O)c1 | CCCCC | 1.57 | 1.24 | 1.10 | 1.94 | | 1.51 | 1.56 | 2.14 | 2.01 | [61] |
| 1580 | Cc1ccccc(O)c1 | CCCCCC | 1.79 | 1.43 | 1.29 | 2.12 | | 1.68 | 1.38 | 2.25 | 2.15 | [61 , 47] |
| 1581 | Cc1ccccc(O)c1 | C1CCCCC1 | 1.47 | 1.11 | 1.08 | 1.46 | | 1.08 | 0.52 | 1.54 | 1.73 | [61 , 47] |
| 1582 | Cc1ccccc(O)c1 | CCCCCCC | 2.00 | 1.59 | 1.46 | 2.29 | | 1.84 | 1.20 | 2.40 | 2.30 | [61] |
| 1583 | Cc1ccccc(O)c1 | CCCCCCCC | 2.20 | 1.73 | 1.62 | 2.47 | | 2.03 | 1.12 | 2.56 | 2.47 | [61] |
| 1584 | Cc1ccccc(O)c1 | c1ccccc1 | 0.48 | 0.34 | 0.36 | 0.65 | | 0.55 | 0.00 | -0.02 | 0.79 | [47 , 61] |
| 1585 | Cc1ccccc(O)c1 | Cc1ccccc1 | 0.72 | 0.57 | 0.57 | 0.78 | | 0.66 | 0.12 | 0.07 | 0.85 | [61] |
| 1586 | Cc1ccccc(O)c1 | CC=C(C)C | 1.06 | 1.04 | 0.83 | 1.51 | | 0.75 | 1.30 | | 1.49 | [61 , 47] |
| 1587 | Cc1ccccc(O)c1 | CC(=C)C=C | 0.74 | 0.46 | 0.38 | 0.77 | | | | | 1.18 | [61 , 47] |
| 1588 | CO | CCO | -0.04 | 0.25 | 0.38 | -0.03 | 0.51 | -0.04 | 0.05 | 0.40 | 0.29 | [161 , 61] |
| 1589 | CO | CCCO | 0.14 | 0.30 | 0.56 | 0.05 | 0.57 | 0.18 | 0.34 | 0.52 | 0.67 | [161] |
| 1590 | CO | CCCCO | 0.27 | 0.37 | 0.77 | 0.17 | 0.70 | 0.43 | 0.63 | 0.47 | 0.77 | [161] |
| 1591 | CO | CCCCCO | 0.52 | 0.46 | 1.02 | 0.31 | 0.93 | 0.70 | 0.94 | 0.62 | 1.26 | [161] |
| 1592 | CO | CCCCCCO | 0.69 | 0.55 | 1.28 | 0.48 | 1.20 | 1.03 | 1.19 | 0.65 | 1.33 | [161] |
| 1593 | CO | CCCCCCCO | 0.92 | 0.65 | 1.55 | 0.66 | 1.68 | 1.38 | 1.35 | | 1.44 | [161] |
| 1594 | CO | C1COCCO1 | 0.24 | 0.23 | 0.48 | 1.48 | 0.29 | 1.96 | 1.32 | 1.02 | 1.22 | [61] |
| 1595 | CO | CC(C)=O | 0.05 | 0.67 | 0.74 | 0.72 | 0.76 | 0.97 | 1.47 | 0.94 | 0.64 | [96 , 161 , 61 , 123] |
| 1596 | CO | CCC(C)=O | 0.11 | 0.78 | 0.94 | 0.82 | 0.92 | 1.62 | 1.79 | 0.94 | 0.59 | [161 , 61] |
| 1597 | CO | CCCC(C)=O | 0.28 | 0.90 | 1.17 | 0.96 | 1.06 | 2.12 | 2.07 | 1.16 | 0.45 | [161] |
| 1598 | CO | CCCCC(C)=O | 0.52 | 1.02 | 1.43 | 1.13 | 2.34 | | | | 0.55 | [161] |
| 1599 | CO | CCCCCC(C)=O | 0.72 | 1.16 | 1.72 | 1.31 | 2.43 | 3.17 | 2.34 | | 0.70 | [161] |
| 1600 | CO | ClCCl | 0.77 | 1.06 | 1.04 | 1.06 | 1.00 | 1.20 | 1.37 | 1.61 | 0.90 | [61 , 123] |
| 1601 | CO | ClC(Cl)Cl | 1.11 | 0.90 | 0.88 | 0.82 | 0.91 | 1.82 | | 1.56 | 0.85 | [61 , 123] |
| 1602 | CO | ClC(Cl)(Cl)Cl | 2.87 | 1.88 | 2.00 | 2.05 | 2.58 | 3.77 | 2.26 | 2.51 | 2.03 | [61 , 123] |
| 1603 | CO | CCN(CC)CC | 0.25 | 0.62 | 1.10 | 0.75 | 0.74 | 5.23 | 2.27 | 1.24 | -0.02 | [61] |
| 1604 | CC(=O)OC | CCCCC | 1.55 | 1.46 | 1.46 | 1.39 | 1.46 | 0.67 | 0.72 | 1.51 | 1.53 | [54] |
| 1605 | CC(=O)OC | CCCCCC | 1.75 | 1.64 | 1.67 | 1.61 | 1.66 | 0.78 | 0.62 | 1.72 | 1.77 | [54] |
| 1606 | CC(=O)OC | C1CCCCC1 | 1.52 | 1.53 | 1.42 | 1.67 | 1.45 | 0.62 | 0.12 | 1.84 | 1.66 | [54] |
| 1607 | CC(=O)OC | CCCC(C)C | 1.68 | 1.64 | 1.67 | 1.61 | 1.66 | | | 1.67 | 1.71 | [54] |
| 1608 | CC(=O)OC | CCCCCCC | 1.95 | 1.80 | 1.87 | 1.83 | 1.85 | 0.89 | 0.51 | 1.92 | 1.96 | [54] |
| 1609 | CC(=O)OC | CC(C)CC(C)C | 1.80 | 1.80 | 1.87 | 1.83 | 1.81 | | | 1.81 | 1.84 | [54] |
| 1610 | CC(=O)OC | CCCCCCCC | 2.14 | 1.95 | 2.07 | 2.05 | 2.08 | 1.01 | 0.47 | 2.10 | 2.14 | [54] |
| 1611 | CC(=O)OC | CC(C)C(C)C(C)C | 1.87 | 1.95 | 2.06 | 2.05 | 1.75 | | | | 1.93 | [54] |
| 1612 | CC(=O)OC | CC(C)CCC(C)C | 2.01 | 1.95 | 2.06 | 2.05 | | | | | 2.01 | [54] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1613 | CC(=O)OC | CCC1CCCCC1 | 1.85 | 1.88 | 1.82 | 2.03 | | | | 2.18 | 2.01 | [54] |
| 1614 | CC(=O)OC | CCCCCCCCC | 2.32 | 2.08 | 2.26 | 2.27 | 2.40 | 1.12 | 0.43 | 2.29 | 2.34 | [54] |
| 1615 | CCCCOC | C1CCCCC1 | 0.21 | 0.42 | 0.36 | 0.27 | | | | | 0.30 | [57] |
| 1616 | CCCCOC | CCCC#CC | -0.04 | -0.04 | -0.05 | -0.08 | | | | | 0.01 | [151] |
| 1617 | CC1CCCCC1 | C1CCCCC1 | 0.00 | -0.01 | -0.01 | 0.00 | -0.16 | -0.22 | -0.21 | -0.01 | 0.01 | [131] |
| 1618 | CC1CCCCC1 | c1ccccc1 | 0.48 | 0.36 | 0.37 | 0.46 | 0.41 | -0.17 | 0.02 | 0.42 | 0.57 | [78] |
| 1619 | CC1CCCCC1 | Cc1ccccc1 | 0.48 | 0.39 | 0.36 | 0.39 | 0.35 | -0.12 | -0.01 | 0.39 | 0.45 | [78] |
| 1620 | CC1CCCC1 | c1ccccc1 | 0.51 | 0.40 | 0.39 | 0.50 | | | | 0.46 | 0.55 | [78 , 108] |
| 1621 | CC1CCCC1 | Cc1ccccc1 | 0.50 | 0.40 | 0.37 | 0.41 | | | | 0.41 | 0.46 | [78] |
| 1622 | ClCCl | C1CCCCC1 | 0.82 | 0.77 | 0.82 | 1.15 | 1.55 | 0.44 | 0.14 | 1.13 | 1.08 | [54 , 61 , 61] |
| 1623 | ClCCl | CCCC(C)C | 0.94 | 0.78 | 0.95 | 1.03 | 1.87 | | | 1.35 | 1.25 | [54 , 61 , 61] |
| 1624 | ClCCl | CCCCCCC | 1.04 | 0.78 | 1.04 | 1.14 | 1.99 | 0.92 | 0.46 | 1.31 | 1.26 | [54 , 61 , 61] |
| 1625 | ClCCl | CC(C)CC(C)C | 0.96 | 0.78 | 1.04 | 1.14 | 1.99 | | | 1.45 | 1.28 | [54 , 61] |
| 1626 | ClCCl | CCCCCCCC | 1.10 | 0.76 | 1.12 | 1.26 | 2.18 | 0.99 | 0.43 | 1.35 | 1.40 | [54 , 61 , 61 , 61] |
| 1627 | ClCCl | CC(C)C(C)C(C)C | 0.96 | 0.76 | 1.12 | 1.26 | 1.87 | | | | 1.28 | [54 , 61 , 61] |
| 1628 | ClCCl | CC(C)CCC(C)C | 1.04 | 0.76 | 1.12 | 1.26 | | | | | 1.33 | [54] |
| 1629 | ClCCl | CCC1CCCCC1 | 0.93 | 0.79 | 1.00 | 1.35 | | | | 1.28 | 1.25 | [54 , 61 , 61] |
| 1630 | ClCCl | CCCCCCCCC | 1.15 | 0.73 | 1.21 | 1.39 | 2.44 | 1.06 | 0.39 | 1.38 | 1.50 | [54 , 61 , 61] |
| 1631 | ClCCl | CCC(C)CCC(C)C | 1.08 | 0.73 | 1.20 | 1.39 | | | | | 1.36 | [61] |
| 1632 | C(I)I | CCO | 3.15 | 2.57 | 2.41 | 2.68 | | | | 3.87 | 3.48 | [61] |
| 1633 | C(I)I | C1COCCO1 | -0.21 | 0.97 | 0.74 | -1.77 | | | | 0.00 | 0.45 | [61] |
| 1634 | C(I)I | CCC(C)=O | -0.13 | 0.66 | 0.70 | 0.63 | | | | 0.56 | 1.36 | [61] |
| 1635 | CCSC | C1CCCCC1 | 0.57 | 0.41 | 0.44 | 0.53 | | | | | 0.60 | [134 , 133] |
| 1636 | CCSC | CCCCCCC | 0.72 | 0.44 | 0.55 | 0.75 | | | | | 0.62 | [134 , 133] |
| 1637 | CC(C)(C)OC | CCCCC#C | -0.49 | -0.07 | -0.11 | -0.07 | | | | | -0.15 | [162] |
| 1638 | NCCO | CCCCC | 3.74 | 2.68 | 2.57 | 4.38 | | 4.90 | 6.79 | | 5.95 | [163] |
| 1639 | NCCO | C1CCCC1 | 3.23 | 2.39 | 2.10 | 3.47 | | 3.41 | 5.22 | | 4.79 | [163] |
| 1640 | NCCO | CCCCCC | 4.27 | 3.10 | 2.97 | 4.85 | | 5.53 | 6.48 | | 6.31 | [163] |
| 1641 | NCCO | C1CCCCC1 | 3.68 | 2.83 | 2.51 | 4.16 | | 4.37 | 5.03 | | 5.20 | [163] |
| 1642 | NCCO | CCCCCCC | 4.80 | 3.49 | 3.36 | 5.33 | | 6.17 | 6.17 | | 6.55 | [164 , 163] |
| 1643 | NCCO | C1CCCCCC1 | 4.07 | 3.24 | 2.90 | 4.83 | | | | | 5.48 | [163] |
| 1644 | NCCO | CCCCCCCC | 5.32 | 3.86 | 3.74 | 5.80 | | 6.82 | 6.03 | | 7.07 | [163] |
| 1645 | NCCO | C1CCCCCCC1 | 4.40 | 3.63 | 3.29 | 5.48 | | 5.57 | 4.43 | | 5.84 | [163] |
| 1646 | NCCO | CCCCCCCCC | 5.83 | 4.23 | 4.12 | 6.27 | | 7.49 | 5.88 | | 7.38 | [163] |
| 1647 | NCCO | c1ccccc1 | 2.11 | 1.75 | 1.30 | 2.46 | | 3.20 | 3.86 | | 2.87 | [164 , 163] |
| 1648 | NCCO | Cc1ccccc1 | 2.63 | 2.28 | 1.77 | 3.26 | | 3.59 | 4.11 | | 3.38 | [163] |
| 1649 | NCCO | Cc1cccc(C)c1 | 3.09 | 2.74 | 2.19 | 4.07 | | 3.97 | 4.17 | | 4.02 | [163] |
| 1650 | NCCO | Cc1ccc(C)cc1 | 3.10 | 2.74 | 2.19 | 4.07 | | 3.93 | 4.29 | | 3.99 | [163] |
| 1651 | NCCO | Cc1ccccc1C | 2.97 | 2.74 | 2.19 | 4.07 | | 3.87 | 4.17 | | 3.86 | [163] |
| 1652 | NCCO | CCCCC=C | 3.52 | 3.04 | 2.90 | 4.38 | | 5.10 | 6.60 | | 5.46 | [163] |
| 1653 | NCCO | CCCCCC=C | 4.01 | 3.43 | 3.28 | 4.86 | | 4.80 | 6.20 | | 5.86 | [163] |
| 1654 | NCCO | CCCCCCC=C | 4.58 | 3.80 | 3.65 | 5.34 | | 5.21 | 6.00 | | 6.31 | [163] |
| 1655 | NCCO | CCCCC#C | 2.27 | 2.50 | 2.37 | 3.85 | | | | | 3.69 | [163] |
| 1656 | NCCO | CCCCCC#C | 2.77 | 2.78 | 2.66 | 4.29 | | | | | 4.19 | [163] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1657 | NCCO | CCCCCCC#C | 3.26 | 3.06 | 2.95 | 4.73 | | | | | 4.71 | [163] |
| 1658 | Cc1cccc(C)c1 | C1CCCCC1 | 0.31 | 0.18 | 0.17 | 0.37 | 0.32 | -0.14 | -0.15 | | 0.39 | [130] |
| 1659 | CCCCCCCCCCCC(=O)N(CC)CC | CCCCC | | -0.21 | -0.01 | 0.17 | | | | | 0.21 | [165] |
| 1660 | CCCCCCCCCCCC(=O)N(CC)CC | CCCCCC | | -0.08 | 0.08 | 0.22 | | | | | 0.27 | [165] |
| 1661 | CCCCCCCCCCCC(=O)N(CC)CC | C1CCCCC1 | | -0.20 | 0.01 | 0.17 | | | | | 0.01 | [165] |
| 1662 | CCCCCCCCCCCC(=O)N(CC)CC | CCCCCCC | | 0.03 | 0.16 | 0.25 | | | | | 0.31 | [165] |
| 1663 | CCCCCCCCCCCC(=O)N(CC)CC | c1ccccc1 | | -0.89 | -0.65 | -0.25 | | | | | -0.51 | [165] |
| 1664 | CCCCCCCCCCCC(=O)N(CC)CC | CO | | 0.45 | 0.90 | 0.17 | | | | | -0.39 | [165] |
| 1665 | CCCCCCCCCCCC(=O)N(CC)CC | CCOC(=O)C | | -0.15 | 0.05 | 0.27 | | | | | 0.15 | [165] |
| 1666 | CCCCCCCCCCCC(=O)N(CC)CC | C1CCOC1 | | -0.40 | -0.22 | -0.31 | | | | | -0.42 | [165] |
| 1667 | CCCCCCCCCCCC(=O)N(CC)CC | CCOCC | | -0.49 | -0.27 | 0.03 | | | | | -0.04 | [165] |
| 1668 | CCCCCCCCCCCC(=O)N(CC)CC | CC(C)=O | | 0.05 | 0.36 | 0.29 | | | | | 0.13 | [165] |
| 1669 | CCCCCCCCCCCC(=O)N(CC)CC | ClCCl | | -0.94 | -0.54 | -0.63 | | | | | -1.43 | [165] |
| 1670 | CCCCCCCCCCCC(=O)N(CC)CC | ClC(Cl)(Cl)Cl | | -1.27 | -1.02 | -0.94 | | | | | -0.58 | [165] |
| 1671 | CN(C)C(C)=O | CCCCC | 1.90 | 1.81 | 1.81 | 2.01 | 1.56 | 1.65 | 2.01 | 2.17 | 2.17 | [54 , 61 , 61 , 74] |
| 1672 | CN(C)C(C)=O | CCCCCC | 2.19 | 2.09 | 2.09 | 2.15 | 1.58 | 1.86 | 1.81 | 2.37 | 2.43 | [54 , 61] |
| 1673 | CN(C)C(C)=O | C1CCCCC1 | 1.86 | 1.82 | 1.76 | 1.97 | 1.44 | 1.36 | 0.89 | 1.98 | 2.08 | [54 , 61 , 61] |
| 1674 | CN(C)C(C)=O | CCCC(C)C | 2.12 | 2.09 | 2.09 | 2.15 | 1.64 | | | 2.45 | 2.38 | [54 , 61 , 61] |
| 1675 | CN(C)C(C)=O | CCCCCCC | 2.47 | 2.35 | 2.37 | 2.29 | 1.60 | 2.07 | 1.62 | 2.58 | 2.65 | [54 , 61 , 61] |
| 1676 | CN(C)C(C)=O | CC(C)CC(C)C | 2.31 | 2.34 | 2.37 | 2.29 | 1.68 | | | 2.74 | 2.60 | [54 , 61 , 61] |
| 1677 | CN(C)C(C)=O | CCCCCCCC | 2.75 | 2.59 | 2.64 | 2.43 | 1.65 | 2.30 | 1.54 | 2.80 | 2.90 | [54 , 61 , 61 , 61] |
| 1678 | CN(C)C(C)=O | CC(C)C(C)C(C)C | 2.45 | 2.58 | 2.64 | 2.43 | 1.39 | | | | 2.66 | [54 , 61 , 61] |
| 1679 | CN(C)C(C)=O | CC(C)CCC(C)C | 2.62 | 2.59 | 2.64 | 2.43 | | | | | 2.85 | [54] |
| 1680 | CN(C)C(C)=O | CCC1CCCCC1 | 2.36 | 2.36 | 2.32 | 2.17 | | | | 2.53 | 2.53 | [54 , 61 , 61] |
| 1681 | CN(C)C(C)=O | CCCCCCCCC | 3.02 | 2.82 | 2.91 | 2.56 | 1.79 | 2.53 | 1.45 | 3.01 | 3.15 | [54 , 61 , 61] |
| 1682 | CN(C)C(C)=O | CCC(C)CCC(C)C | 2.86 | 2.82 | 2.90 | 2.56 | | | | | 2.75 | [61] |
| 1683 | CN(C)C(C)=O | c1ccccc1 | 0.32 | -0.25 | -0.37 | 0.05 | 0.64 | 0.92 | 0.28 | 0.17 | 0.36 | [61] |
| 1684 | CN(C)C(C)=O | Cc1ccccc1 | 0.63 | -0.30 | -0.46 | 0.34 | 0.55 | 0.96 | 0.42 | 0.43 | 0.47 | [61] |
| 1685 | CN(C)C(C)=O | CCCC=C | 1.21 | 1.31 | 1.31 | 1.56 | 1.44 | 1.01 | 2.01 | 1.58 | 1.60 | [74] |
| 1686 | CN(C)C(C)=O | CCO | -1.24 | -1.43 | -1.51 | -0.51 | 0.28 | 0.00 | 0.39 | -0.97 | -0.69 | [61] |
| 1687 | CN(C)C(C)=O | C1COCCO1 | 0.19 | 0.22 | 0.01 | 0.15 | -0.11 | 0.41 | -0.12 | 0.12 | 0.17 | [61] |
| 1688 | CN(C)C(C)=O | CCC(C)=O | 0.04 | 0.06 | 0.06 | -0.26 | 0.39 | -0.01 | 0.15 | 0.17 | 0.14 | [61] |
| 1689 | CN(C)C=O | CCCCCC | 2.63 | 2.62 | 2.65 | 2.76 | 2.21 | 2.60 | 2.95 | 2.86 | 2.97 | [59 , 59 , 147 , 54 , 61 , 61 , 61 , 47] |
| 1690 | CN(C)C=O | c1ccccc1 | 0.59 | 0.44 | 0.27 | 0.53 | 0.86 | 1.34 | 1.07 | 0.67 | 0.34 | [59 , 59 , 47 , 73] |
| 1691 | CN(C)C=O | CCCCC | 2.29 | 2.29 | 2.30 | 2.54 | 2.12 | 2.32 | 3.18 | 2.63 | 2.64 | [54 , 61 , 61 , 61] |
| 1692 | CN(C)C=O | C1CCCCC1 | 2.25 | 2.30 | 2.24 | 2.50 | 2.04 | 1.92 | 1.87 | 2.42 | 2.65 | [147 , 54 , 61 , 61 , 61] |
| 1693 | CN(C)C=O | CCCC(C)C | 2.54 | 2.61 | 2.65 | 2.76 | 2.25 | | | 2.96 | 2.96 | [54 , 61 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1694 | CN(C)C=O | CC1CCCC1 | 2.26 | 2.30 | 2.24 | 2.25 | 1.87 | | | 2.47 | 2.51 | [61] |
| 1695 | CN(C)C=O | CCCCCCC | 2.96 | 2.92 | 2.99 | 2.98 | 2.30 | 2.88 | 2.73 | 3.12 | 3.35 | [147 , 54 , 61 , 61 , 61] |
| 1696 | CN(C)C=O | CC(C)CC(C)C | 2.77 | 2.92 | 2.99 | 2.98 | 2.33 | | | 3.29 | 3.24 | [54 , 61 , 61 , 61] |
| 1697 | CN(C)C=O | C1CCCCCC1 | 2.50 | 2.63 | 2.59 | 2.85 | 1.96 | | | 2.71 | 2.91 | [147] |
| 1698 | CN(C)C=O | CC1CCCCC1 | 2.53 | 2.63 | 2.59 | 2.60 | 2.05 | 2.23 | 2.29 | 2.75 | 2.75 | [61] |
| 1699 | CN(C)C=O | CCCCCCCC | 3.28 | 3.21 | 3.33 | 3.20 | 2.43 | 3.18 | 2.62 | 3.37 | 3.61 | [147 , 54 , 61 , 61 , 61 , 61] |
| 1700 | CN(C)C=O | C1CCCCCCC1 | 2.71 | 2.94 | 2.93 | 3.19 | 2.03 | 2.48 | 1.48 | 2.99 | 3.25 | [147] |
| 1701 | CN(C)C=O | CC(C)CC(C)(C)C | 2.96 | 3.25 | 3.38 | 3.20 | 2.37 | 3.52 | 3.49 | 3.62 | 3.35 | [61] |
| 1702 | CN(C)C=O | CC(C)C(C)C(C)C | 2.93 | 3.21 | 3.32 | 3.20 | 2.14 | | | | 3.35 | [54 , 61 , 61 , 61] |
| 1703 | CN(C)C=O | CC(C)CCC(C)C | 3.13 | 3.21 | 3.33 | 3.20 | | | | | 3.34 | [54] |
| 1704 | CN(C)C=O | CCC1CCCCC1 | 2.84 | 2.93 | 2.93 | 2.84 | | | | 3.04 | 3.19 | [54 , 61 , 61 , 61] |
| 1705 | CN(C)C=O | CCCCCCCCC | 3.60 | 3.49 | 3.67 | 3.42 | 2.64 | 3.48 | 2.52 | 3.61 | 3.99 | [54 , 61 , 61 , 61] |
| 1706 | CN(C)C=O | CCC(C)CCC(C)C | 3.41 | 3.49 | 3.66 | 3.42 | | | | | 3.73 | [61 , 61] |
| 1707 | CN(C)C=O | Cc1ccccc1 | 0.92 | 0.63 | 0.44 | 0.78 | 0.85 | 1.41 | 1.24 | 0.93 | 0.65 | [61] |
| 1708 | CN(C)C=O | CCCC=C | 1.54 | 1.90 | 1.90 | 1.78 | 1.92 | 1.57 | 3.19 | 2.03 | 2.05 | [61] |
| 1709 | CN(C)C=O | CCCCC=C | 1.88 | 2.22 | 2.24 | 2.02 | 1.97 | 2.31 | 3.05 | 2.36 | 2.31 | [147 , 61] |
| 1710 | CN(C)C=O | C1CCC=CC1 | 1.58 | 1.98 | 1.89 | 1.66 | 1.64 | 1.10 | 1.33 | | 1.76 | [61] |
| 1711 | CN(C)C=O | CCCCCC=C | 2.18 | 2.53 | 2.58 | 2.25 | 2.00 | 2.11 | 2.74 | | 2.56 | [147 , 61] |
| 1712 | CN(C)C=O | CCCCCCC=C | 2.54 | 2.82 | 2.91 | 2.48 | 2.14 | 2.29 | 2.60 | 2.69 | 2.83 | [147 , 61] |
| 1713 | CN(C)C=O | CCCCC#C | 0.46 | 0.37 | 0.44 | 0.77 | | | | | 0.84 | [147] |
| 1714 | CN(C)C=O | CCCCCC#C | 0.75 | 0.57 | 0.69 | 0.95 | | | | | 1.12 | [147] |
| 1715 | CN(C)C=O | CCCCCCC#C | 1.04 | 0.77 | 0.94 | 1.14 | | | | | 1.38 | [147] |
| 1716 | CCCCCCCCCCCCCCCCBr | Cc1cccc(C)c1 | | -0.07 | 0.05 | -0.42 | | | | | -0.27 | [61] |
| 1717 | CCCCCCCCCCCCCCCCBr | Cc1ccc(C)cc1 | | -0.07 | 0.05 | -0.42 | | | | | -0.30 | [61] |
| 1718 | CCCCCCCCCCCCCCCCBr | CCc1ccccc1 | | -0.20 | -0.06 | -0.26 | | | | | -0.22 | [61] |
| 1719 | CCCCCCCCCCCCCCCCBr | CCCc1ccccc1 | | -0.14 | -0.04 | -0.22 | | | | | -0.17 | [61] |
| 1720 | CCCCCCCCCCCCCCCCBr | Cc1cc(C)cc(C)c1 | | 0.04 | 0.11 | -0.49 | | | | | -0.26 | [61] |
| 1721 | CCCCCCCCCCCCCCCCBr | CC(C)c1ccccc1 | | -0.19 | -0.09 | -0.19 | | | | | -0.15 | [61] |
| 1722 | CCCC=O | C1CCCCC1 | 1.09 | 1.06 | 1.00 | 1.17 | | 0.45 | -0.06 | 1.18 | 1.13 | [71] |
| 1723 | CCCCO | CCCCC | 1.33 | 1.15 | 1.10 | 1.44 | 1.56 | 1.89 | 2.72 | 1.58 | 1.44 | [166 , 54 , 61 , 61 , 61] |
| 1724 | CCCCO | CCCCCC | 1.52 | 1.35 | 1.28 | 1.57 | 1.74 | 2.15 | 2.49 | 1.76 | 1.61 | [166 , 54 , 61 , 61 , 61 , 167 , 76] |
| 1725 | CCCCO | CCCCCCC | 1.69 | 1.52 | 1.44 | 1.69 | 1.91 | 2.42 | 2.26 | 1.93 | 1.75 | [166 , 54 , 61 , 61 , 61 , 63] |
| 1726 | CCCCO | CCCCCCCC | 1.86 | 1.68 | 1.60 | 1.81 | 2.13 | 2.70 | 2.16 | 2.10 | 1.87 | [166 , 54 , 61 , 61 , 61 , 167] |
| 1727 | CCCCO | C1CCCCC1 | 1.32 | 1.28 | 1.08 | 1.47 | 1.61 | 1.67 | 1.40 | 1.65 | 1.44 | [54 , 61 , 61 , 61 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1728 | CCCCO | CCCC(C)C | 1.46 | 1.35 | 1.28 | 1.57 | 1.75 | | | 1.78 | 1.61 | [54 , 61 , 61] |
| 1729 | CCCCO | CC(C)CC(C)C | 1.58 | 1.52 | 1.44 | 1.69 | 1.89 | | | 1.97 | 1.72 | [54 , 61 , 61] |
| 1730 | CCCCO | CC(C)C(C)C(C)C | 1.66 | 1.69 | 1.60 | 1.81 | 1.81 | | | | 1.78 | [54 , 61 , 61] |
| 1731 | CCCCO | CC(C)CCC(C)C | 1.76 | 1.68 | 1.60 | 1.81 | | | | | 1.85 | [54] |
| 1732 | CCCCO | CCC1CCCCC1 | 1.64 | 1.65 | 1.41 | 1.65 | | | | 2.03 | 1.76 | [54 , 61 , 61] |
| 1733 | CCCCO | CCCCCCCCC | 2.03 | 1.83 | 1.76 | 1.93 | 2.43 | 2.98 | 2.06 | 2.28 | 2.13 | [54 , 61 , 61] |
| 1734 | CCCCO | CCC(C)CCC(C)C | 1.91 | 1.83 | 1.76 | 1.93 | | | | | 1.83 | [61] |
| 1735 | CCCCO | c1ccccc1 | 0.92 | 1.05 | 0.76 | 1.18 | 1.16 | 1.12 | 0.65 | 1.04 | 1.07 | [61 , 61 , 47] |
| 1736 | CCCCO | Cc1ccccc1 | 1.12 | 1.19 | 0.83 | 1.21 | 1.25 | 1.29 | 0.82 | 1.21 | 1.23 | [61] |
| 1737 | CCCCO | CCCC=C | 1.04 | 1.19 | 1.14 | 1.25 | 1.36 | 1.04 | 2.72 | 1.42 | 1.24 | [61] |
| 1738 | CCCCO | CC(C)C=C | 1.02 | 1.19 | 1.14 | 1.25 | | | | | 1.21 | [61] |
| 1739 | CCCCO | CC(=C)C=C | 0.96 | 1.18 | 1.15 | 0.92 | 1.21 | | | | 1.05 | [61] |
| 1740 | CCCCO | CCCCC=C | 1.23 | 1.39 | 1.31 | 1.39 | 1.51 | 1.99 | 2.58 | 1.63 | 1.55 | [61] |
| 1741 | CCCCN | CCCCCCC | 1.02 | 0.75 | 0.78 | 0.87 | | 0.66 | 0.14 | | 0.89 | [137] |
| 1742 | CCCCN | CCc1ccccc1 | 0.47 | 0.39 | 0.24 | 0.49 | | 0.36 | -0.14 | | 0.41 | [168] |
| 1743 | CCCCCl | CCCCl | 0.00 | -0.01 | 0.00 | 0.01 | | | | | 0.02 | [61] |
| 1744 | CCCCCl | CC(C)(C)Cl | 0.01 | 0.04 | 0.04 | 0.06 | | | | | 0.00 | [61] |
| 1745 | CCCCCl | ClCCl | -0.06 | 0.06 | 0.11 | 0.08 | | | | | 0.02 | [61] |
| 1746 | CCCCCl | ClC(Cl)Cl | -0.08 | -0.02 | -0.01 | -0.11 | | | | | -0.07 | [61] |
| 1747 | CCCCCl | CCBr | 0.12 | 0.02 | 0.06 | -0.11 | | | | | 0.02 | [61] |
| 1748 | CCCCCl | C[N+](=O)[O-] | 1.45 | 1.41 | 1.46 | 1.45 | | | | | 1.65 | [61] |
| 1749 | CCCCCl | CCI | 0.17 | 0.19 | 0.20 | 0.13 | | | | | 0.25 | [61] |
| 1750 | CCCCCl | C(=S)=S | 0.57 | 0.63 | 0.68 | 0.49 | | | | | 0.44 | [61] |
| 1751 | CCCCCCCCCCCCCCCCCl | CCCCC | -0.07 | -0.40 | -0.20 | -0.09 | | | | | 0.01 | [61] |
| 1752 | CCCCCCCCCCCCCCCCCl | CCCCCC | -0.02 | -0.30 | -0.14 | -0.06 | | | | | 0.09 | [61] |
| 1753 | CCCCCCCCCCCCCCCCCl | c1ccccc1 | -0.02 | -0.33 | -0.07 | -0.21 | | | | | -0.05 | [61] |
| 1754 | CCCCCCCCCCCCCCCCCl | Cc1cccc(C)c1 | -0.01 | -0.21 | -0.09 | -0.29 | | | | | -0.27 | [61] |
| 1755 | CCCCCCCCCCCCCCCCCl | Cc1ccc(C)cc1 | -0.02 | -0.21 | -0.09 | -0.29 | | | | | -0.30 | [61] |
| 1756 | CCCCCCCCCCCCCCCCCl | Cc1ccccc1C | 0.00 | -0.21 | -0.09 | -0.29 | | | | | -0.26 | [61] |
| 1757 | CCCCCCCCCCCCCCCCCl | CCc1ccccc1 | 0.04 | -0.19 | -0.06 | -0.22 | | | | | -0.20 | [61] |
| 1758 | CCCCCCCCCCCCCCCCCl | CCCc1ccccc1 | 0.04 | -0.14 | -0.05 | -0.19 | | | | | -0.16 | [61] |
| 1759 | CCCCCCCCCCCCCCCCCl | Cc1cc(C)cc(C)c1 | -0.11 | -0.24 | -0.16 | -0.33 | | | | | -0.24 | [61] |
| 1760 | CCCCCCCCCCCCCCCCCl | CC(C)c1ccccc1 | 0.03 | -0.15 | -0.06 | -0.16 | | | | | -0.13 | [61] |
| 1761 | CCCCCCCCCCCCCCCCCl | CCCC=C | -0.19 | -0.46 | -0.24 | -0.21 | | | | | -0.08 | [61] |
| 1762 | CCCCCCCCCCCCCCCCCl | CCCCC=C | -0.13 | -0.37 | -0.19 | -0.16 | | | | | -0.05 | [61] |
| 1763 | CCCCCCCCCCCCCCCCCl | CCCCCC=C | -0.11 | -0.29 | -0.15 | -0.13 | | | | | -0.02 | [61] |
| 1764 | CCCCCCCCCC | CCCCC | -0.06 | -0.15 | -0.07 | -0.04 | -0.05 | -0.31 | -0.25 | -0.06 | -0.13 | [54 , 61 , 61] |
| 1765 | CCCCCCCCCC | CCCCCC | -0.03 | -0.09 | -0.04 | -0.02 | 0.01 | -0.29 | -0.26 | -0.06 | -0.03 | [54 , 61 , 61] |
| 1766 | CCCCCCCCCC | C1CCCCC1 | -0.06 | -0.13 | -0.06 | -0.01 | -0.12 | -0.36 | -0.29 | -0.13 | -0.07 | [54 , 61 , 61 , 128] |
| 1767 | CCCCCCCCCC | CCCC(C)C | -0.04 | -0.09 | -0.04 | -0.02 | 0.05 | | | 0.00 | -0.02 | [54 , 61 , 61] |
| 1768 | CCCCCCCCC | CCCCCC | -0.02 | -0.04 | -0.02 | -0.01 | 0.07 | -0.27 | -0.26 | -0.05 | -0.03 | [54 , 61 , 61] |
| 1769 | CCCCCCCCC | CC(C)CC(C)C | -0.02 | -0.05 | -0.02 | -0.01 | 0.12 | | | 0.06 | 0.02 | [54 , 61 , 61] |
| 1770 | CCCCCCCCC | CCCCCCC | -0.01 | -0.02 | -0.01 | -0.01 | 0.17 | -0.24 | -0.24 | -0.03 | 0.03 | [54 , 61 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1771 | CCCCCCCCCC | CC(C)C(C)C(C)C | -0.01 | -0.02 | -0.01 | -0.01 | -0.11 | | | | -0.01 | [54 , 61 , 61] |
| 1772 | CCCCCCCCCC | CC(C)CCC(C)C | -0.01 | -0.02 | -0.01 | -0.01 | | | | | 0.06 | [54] |
| 1773 | CCCCCCCCCC | CCC1CCCCC1 | -0.02 | -0.02 | -0.02 | 0.01 | | | | -0.04 | 0.01 | [54 , 61 , 61] |
| 1774 | CCCCCCCCCC | CCCCCCCCC | 0.00 | 0.00 | 0.00 | 0.00 | 0.35 | -0.21 | -0.21 | -0.02 | 0.17 | [54 , 61] |
| 1775 | CCCCCCCCCC | CCC(C)CCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | | | | | 0.05 | [61] |
| 1776 | CCCCCCCCCC | c1ccccc1 | 0.42 | 0.22 | 0.28 | 0.31 | 0.40 | -0.30 | 0.15 | 0.26 | 0.40 | [169] |
| 1777 | CCCCCCCCCC | Cc1ccccc1 | 0.44 | 0.30 | 0.30 | 0.29 | 0.37 | -0.22 | 0.09 | 0.26 | 0.23 | [61] |
| 1778 | CCCCCCCCCC | CCO | 4.13 | 3.12 | 3.11 | 3.68 | 3.72 | 0.90 | 8.51 | 4.23 | 3.74 | [166] |
| 1779 | CCCCCCCCCC | C1COCCO1 | 1.07 | 1.82 | 1.62 | 0.99 | 1.01 | 0.03 | 1.29 | 1.23 | 1.15 | [166] |
| 1780 | CCCCCCCCCC | CCC(C)=O | 1.58 | 1.50 | 1.60 | 1.50 | 1.45 | 0.11 | 0.41 | 1.30 | 1.42 | [166] |
| 1781 | CCCCCCCCCCO | CCCCCC | 0.62 | 0.46 | 0.52 | 0.75 | 0.90 | 0.75 | 1.96 | | 0.85 | [170] |
| 1782 | CCCCCCCCCCCC | CCCCC | -0.09 | -0.24 | -0.12 | -0.07 | 0.08 | -0.36 | -0.22 | -0.09 | -0.08 | [54 , 61 , 171 , 172 , 172 , 172] |
| 1783 | CCCCCCCCCCCC | C1CCCC1 | -0.14 | -0.31 | -0.16 | -0.12 | -0.16 | -0.49 | -0.49 | -0.30 | -0.14 | [172 , 172 , 172] |
| 1784 | CCCCCCCCCCCC | CCCCCC | -0.06 | -0.16 | -0.08 | -0.05 | 0.14 | -0.33 | -0.26 | -0.09 | -0.01 | [54 , 61 , 171 , 172 , 172 , 172] |
| 1785 | CCCCCCCCCCCC | C1CCCCC1 | -0.09 | -0.21 | -0.11 | -0.06 | -0.08 | -0.43 | -0.40 | -0.22 | -0.08 | [54 , 61 , 128 , 172 , 172 , 172] |
| 1786 | CCCCCCCCCCCC | CCCC(C)C | -0.06 | -0.16 | -0.08 | -0.05 | 0.18 | | | -0.02 | 0.02 | [54 , 61] |
| 1787 | CCCCCCCCCCCC | CCCCCCC | -0.04 | -0.11 | -0.05 | -0.03 | 0.20 | -0.31 | -0.29 | -0.07 | 0.02 | [54 , 61 , 171 , 172 , 172 , 172] |
| 1788 | CCCCCCCCCCCC | CC(C)CC(C)C | -0.04 | -0.11 | -0.05 | -0.03 | 0.25 | | | 0.07 | 0.07 | [54 , 61] |
| 1789 | CCCCCCCCCCCC | CCCCCCCC | -0.02 | -0.06 | -0.03 | -0.02 | 0.31 | -0.29 | -0.27 | -0.05 | 0.04 | [54 , 61] |
| 1790 | CCCCCCCCCCCC | CC(C)C(C)C(C)C | -0.03 | -0.06 | -0.03 | -0.02 | 0.03 | | | | 0.01 | [54 , 61] |
| 1791 | CCCCCCCCCCCC | CC(C)CCC(C)C | -0.02 | -0.06 | -0.03 | -0.02 | | | | | 0.09 | [54] |
| 1792 | CCCCCCCCCCCC | CCC1CCCCC1 | -0.04 | -0.07 | -0.04 | -0.02 | | | | -0.12 | -0.03 | [54 , 61] |
| 1793 | CCCCCCCCCCCC | CCCCCCCCC | -0.01 | -0.03 | -0.02 | -0.01 | 0.49 | -0.26 | -0.25 | -0.04 | 0.06 | [54 , 61] |
| 1794 | CCCCCCCCCCCC | c1ccccc1 | 0.36 | 0.10 | 0.22 | 0.22 | 0.33 | -0.40 | 0.03 | 0.16 | 0.25 | [172 , 172 , 172] |
| 1795 | CCCCCCCCCCCCO | CCCCC | 0.38 | 0.12 | 0.28 | 0.52 | | 0.49 | 2.24 | | 0.67 | [61] |
| 1796 | CCCCCCCCCCCCO | CCCCCC | 0.48 | 0.29 | 0.39 | 0.61 | | 0.60 | 1.91 | | 0.76 | [61 , 173] |
| 1797 | CCCCCCCCCCCCO | C1CCCCC1 | 0.36 | 0.18 | 0.29 | 0.50 | | 0.19 | 0.43 | | 0.57 | [61] |
| 1798 | CCCCCCCCCCCCO | CCCCCCC | 0.57 | 0.42 | 0.49 | 0.68 | | 0.70 | 1.61 | | 0.86 | [61] |
| 1799 | CCCCCCCCCCCCO | CC1CCCCC1 | 0.45 | 0.34 | 0.39 | 0.54 | | 0.31 | 0.99 | | 0.64 | [61] |
| 1800 | CCCCCCCCCCCCO | CC(C)CC(C)(C)C | 0.58 | 0.55 | 0.59 | 0.75 | | 1.11 | 2.78 | | 0.71 | [86] |
| 1801 | CCCCCCCCCCCCO | c1ccccc1 | 0.36 | 0.12 | 0.23 | 0.39 | | -0.15 | -0.36 | | 0.81 | [61] |
| 1802 | CCCCCCCCCCCCO | CCCC=C | 0.25 | 0.08 | 0.25 | 0.38 | | 0.08 | 2.23 | | 0.59 | [61] |
| 1803 | CCCCCCCCCCCCO | CCCCC=C | 0.34 | 0.24 | 0.36 | 0.48 | | 0.52 | 2.04 | | 0.71 | [61] |
| 1804 | CCCCCCCCCCCCO | CCCCCC=C | 0.43 | 0.37 | 0.46 | 0.57 | | 0.27 | 1.62 | | 0.79 | [61] |
| 1805 | CCCCCCCCCCCCO | CCCCl | 0.31 | -0.09 | 0.13 | 0.40 | | | | | 0.65 | [61] |
| 1806 | CCCCCCCCCCCCO | CCCCCl | 0.38 | 0.07 | 0.23 | 0.45 | | -0.11 | 0.10 | | 0.70 | [61] |
| 1807 | CC | CC(=O)OC | 1.69 | 1.24 | 1.31 | 1.65 | | | | | 0.94 | [119] |
| 1808 | CCO | CCCCC | 2.14 | 1.80 | 1.66 | 2.15 | 2.18 | 3.14 | 3.04 | 2.40 | 2.14 | [166 , 123 , 54 , 61 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1809 | CCO | CCCCCC | 2.41 | 2.05 | 1.90 | 2.33 | 2.41 | 3.55 | 2.84 | 2.64 | 2.41 | [166 , 47 , 54 , 61 , 61] |
| 1810 | CCO | CCCCCCC | 2.67 | 2.27 | 2.13 | 2.52 | 2.63 | 3.98 | 2.65 | 2.89 | 2.53 | [166 , 54 , 61 , 61 , 174] |
| 1811 | CCO | CCCCCCCC | 2.93 | 2.48 | 2.35 | 2.71 | 2.89 | 4.42 | 2.55 | 3.13 | 2.77 | [166 , 54 , 61 , 61 , 61 , 174] |
| 1812 | CCO | c1ccccc1 | 1.42 | 1.60 | 1.06 | 1.75 | 1.54 | 2.08 | 1.21 | 1.69 | 1.67 | [123 , 47 , 61 , 73 , 80 , 107] |
| 1813 | CCO | C1CCCCC1 | 2.13 | 1.99 | 1.61 | 2.26 | 2.24 | 2.86 | 1.91 | 2.53 | 2.20 | [54 , 61 , 61] |
| 1814 | CCO | CCCC(C)C | 2.33 | 2.05 | 1.90 | 2.33 | 2.40 | | | 2.64 | 2.33 | [54] |
| 1815 | CCO | CC(C)CC(C)C | 2.49 | 2.27 | 2.12 | 2.52 | 2.56 | | | 2.88 | 2.43 | [54 , 61 , 61] |
| 1816 | CCO | CC(C)CC(C)(C)C | 2.60 | 2.46 | 2.39 | 2.70 | 2.68 | 4.61 | 3.29 | 3.10 | 2.63 | [61] |
| 1817 | CCO | CC(C)C(C)C(C)C | 2.61 | 2.48 | 2.35 | 2.71 | 2.55 | | | | 2.58 | [54 , 61 , 61] |
| 1818 | CCO | CC(C)CCC(C)C | 2.77 | 2.48 | 2.35 | 2.71 | | | | | 2.66 | [54] |
| 1819 | CCO | CCC1CCCCC1 | 2.60 | 2.47 | 2.07 | 2.53 | | | | 3.03 | 2.60 | [54 , 61 , 61] |
| 1820 | CCO | CCCCCCCCC | 3.19 | 2.68 | 2.57 | 2.89 | 3.24 | 4.87 | 2.46 | 3.37 | 3.01 | [54 , 61 , 61] |
| 1821 | CCO | CCC(C)CCC(C)C | 3.00 | 2.68 | 2.57 | 2.89 | | | | | 2.61 | [61] |
| 1822 | CCO | Cc1ccccc1 | 1.71 | 1.76 | 1.16 | 1.83 | 1.69 | 2.34 | 1.36 | 1.88 | 1.75 | [61] |
| 1823 | CCN1CCCC1=O | CCCCC | 1.43 | 1.01 | 0.97 | 1.76 | | | | 1.98 | 1.97 | [62] |
| 1824 | CCN1CCCC1=O | CCCCCC | 1.65 | 1.18 | 1.14 | 1.93 | | | | 2.14 | 2.13 | [62] |
| 1825 | CCN1CCCC1=O | C1CCCCC1 | 1.39 | 0.95 | 0.96 | 1.72 | | | | 1.60 | 1.70 | [62] |
| 1826 | CCN1CCCC1=O | CCCCCCC | 1.87 | 1.33 | 1.30 | 2.10 | | | | 2.33 | 2.30 | [62] |
| 1827 | CCN1CCCC1=O | CCCCCCCC | 2.09 | 1.46 | 1.45 | 2.26 | | | | 2.51 | 2.47 | [62] |
| 1828 | CCN1CCCC1=O | c1ccccc1 | 0.10 | -0.60 | -0.60 | -0.13 | | | | -0.06 | -0.15 | [62] |
| 1829 | CCN1CCCC1=O | Cc1ccccc1 | 0.36 | -0.73 | -0.76 | 0.02 | | | | 0.15 | 0.11 | [62] |
| 1830 | CCN1CCCC1=O | CCCC=C | 0.85 | 0.65 | 0.63 | 1.11 | | | | 1.43 | 1.40 | [62] |
| 1831 | CCN1CCCC1=O | CCCCC=C | 1.08 | 0.82 | 0.79 | 1.30 | | | | 1.67 | 1.56 | [62] |
| 1832 | CCN1CCCC1=O | C1CCC=CC1 | 0.88 | 0.66 | 0.67 | 0.92 | | | | | 1.12 | [62] |
| 1833 | CCN1CCCC1=O | CCCCCC=C | 1.29 | 0.97 | 0.94 | 1.48 | | | | | 1.68 | [62] |
| 1834 | CCN1CCCC1=O | CCCCCCC=C | 1.52 | 1.10 | 1.09 | 1.65 | | | | 1.93 | 1.81 | [62] |
| 1835 | CCN1CCCC1=O | C1CCOC1 | 0.19 | 0.19 | 0.10 | 0.43 | | | | 0.20 | 0.25 | [62] |
| 1836 | CCN1CCCC1=O | CC(C)(C)OC | 0.57 | 0.27 | 0.18 | 0.92 | | | | 1.00 | 1.07 | [62] |
| 1837 | CCN1CCCC1=O | CCOC(C)(C)C | 0.77 | 0.57 | 0.49 | 1.24 | | | | | 1.39 | [62] |
| 1838 | CCN1CCCC1=O | CCC(C)(C)OC | 0.78 | 0.38 | 0.29 | 1.06 | | | | | 1.19 | [62] |
| 1839 | CCN1CCCC1=O | CCOCC | 0.48 | 0.25 | 0.19 | 0.94 | | | | 0.99 | 1.05 | [62] |
| 1840 | CCN1CCCC1=O | CC(C)OC(C)C | 0.79 | 0.77 | 0.72 | 1.43 | | | | 1.50 | 1.55 | [62] |
| 1841 | CCN1CCCC1=O | CC(C)=O | -0.07 | 0.02 | 0.01 | -0.13 | | | | 0.11 | 0.20 | [62] |
| 1842 | CCN1CCCC1=O | CCC(C)=O | -0.05 | 0.02 | -0.02 | -0.09 | | | | 0.11 | 0.19 | [62] |
| 1843 | CCN1CCCC1=O | CCCC(C)=O | 0.01 | 0.03 | -0.01 | -0.03 | | | | 0.27 | 0.23 | [62] |
| 1844 | CCN1CCCC1=O | CC=O | -0.12 | -0.24 | -0.19 | -0.08 | | | | -0.08 | 0.08 | [62] |
| 1845 | CCN1CCCC1=O | ClCCl | -1.39 | -0.51 | -0.43 | -0.09 | | | | -1.56 | -1.31 | [62] |
| 1846 | O=CN1CCOCC1 | CCCCCC | 2.82 | 2.37 | 2.36 | 3.20 | | | | 3.71 | 3.95 | [154] |
| 1847 | O=CN1CCOCC1 | C1CCCCC1 | 2.38 | 2.08 | 1.98 | 2.72 | | | | 3.03 | 3.25 | [154] |
| 1848 | O=CN1CCOCC1 | CCCCCCC | 3.19 | 2.69 | 2.68 | 3.49 | | | | 4.09 | 4.19 | [154] |
| 1849 | O=CN1CCOCC1 | CCCCCCCC | 3.55 | 3.00 | 3.00 | 3.78 | | | | 4.47 | 4.55 | [154] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1850 | O=CN1CCOCC1 | CCCCCCCCC | 3.90 | 3.29 | 3.31 | 4.06 | | | | 4.85 | 4.81 | [154] |
| 1851 | O=CN1CCOCC1 | c1ccccc1 | 0.55 | 0.34 | 0.18 | 0.32 | | | | 0.98 | 0.93 | [154] |
| 1852 | O=CN1CCOCC1 | Cc1ccccc1 | 0.92 | 0.65 | 0.44 | 0.52 | | | | 1.40 | 1.30 | [154] |
| 1853 | CCCCCCC | CCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.06 | -0.22 | -0.21 | -0.02 | 0.01 | [73 , 54 , 61] |
| 1854 | CCCCCCC | c1ccccc1 | 0.52 | 0.39 | 0.35 | 0.48 | 0.48 | -0.13 | 0.25 | 0.43 | 0.52 | [73 , 78 , 109 , 110] |
| 1855 | CCCCCCC | CCCCC | -0.01 | -0.04 | -0.02 | 0.00 | -0.02 | -0.25 | -0.22 | -0.02 | -0.05 | [54 , 61] |
| 1856 | CCCCCCC | C1CCCC1 | -0.03 | -0.05 | -0.04 | 0.04 | -0.15 | -0.29 | -0.25 | -0.04 | 0.09 | [125] |
| 1857 | CCCCCCC | C1CCCCC1 | -0.01 | 0.00 | -0.01 | 0.06 | -0.05 | -0.22 | -0.15 | 0.04 | 0.09 | [54 , 128 , 128 , 125 , 130] |
| 1858 | CCCCCCC | CCCC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | 0.10 | | | 0.01 | 0.00 | [54 , 61] |
| 1859 | CCCCCCC | CCCCCCC | 0.00 | 0.00 | 0.00 | 0.00 | 0.12 | -0.20 | -0.20 | 0.00 | 0.05 | [54] |
| 1860 | CCCCCCC | CC(C)CC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | 0.17 | | | 0.06 | 0.04 | [54 , 61] |
| 1861 | CCCCCCC | C1CCCCCC1 | 0.02 | 0.03 | 0.00 | 0.07 | -0.20 | | | 0.16 | 0.20 | [125] |
| 1862 | CCCCCCC | CCCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.23 | -0.16 | -0.16 | 0.01 | 0.05 | [54 , 61 , 61] |
| 1863 | CCCCCCC | C1CCCCCCC1 | 0.04 | 0.04 | 0.00 | 0.06 | -0.24 | -0.03 | 0.12 | 0.25 | 0.26 | [125] |
| 1864 | CCCCCCC | CC(C)C(C)C(C)C | 0.00 | -0.01 | 0.00 | 0.00 | -0.05 | | | | 0.04 | [54 , 61] |
| 1865 | CCCCCCC | CC(C)CCC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | | | | | 0.10 | [54] |
| 1866 | CCCCCCC | CCC1CCCCC1 | 0.01 | 0.04 | 0.00 | 0.08 | | | | 0.07 | 0.09 | [54 , 61] |
| 1867 | CCCCCCC | CCCCCCCCC | -0.01 | -0.03 | -0.01 | 0.00 | 0.42 | -0.14 | -0.14 | 0.02 | 0.06 | [54 , 61] |
| 1868 | CCCCCCC | C1CCCCCCCCC1 | 0.05 | 0.01 | -0.02 | 0.03 | | | | | 0.22 | [125] |
| 1869 | CCCCCCC | Cc1ccccc1 | 0.53 | 0.44 | 0.36 | 0.46 | 0.46 | -0.06 | 0.20 | 0.42 | 0.32 | [61 , 78] |
| 1870 | CCCCCCC | Cc1ccc(C)cc1 | 0.44 | 0.43 | 0.31 | 0.46 | 0.47 | -0.01 | 0.16 | 0.31 | 0.33 | [108] |
| 1871 | CCCCCCC | CCc1ccccc1 | 0.51 | 0.40 | 0.29 | 0.37 | 0.54 | -0.04 | 0.15 | 0.45 | 0.43 | [108] |
| 1872 | CCCCCCC | C=Cc1ccccc1 | 0.69 | 0.55 | 0.44 | 0.66 | 0.90 | | | | 0.33 | [108] |
| 1873 | CCCCCCC | CCCC=C | 0.03 | 0.03 | 0.06 | 0.03 | 0.06 | -0.12 | -0.24 | -0.05 | -0.02 | [61] |
| 1874 | CCCCCCC | CC(C)C=C | 0.03 | 0.03 | 0.06 | 0.03 | | | | | -0.03 | [61] |
| 1875 | CCCCCCC | CC(=C)C=C | 0.27 | 0.11 | 0.17 | 0.29 | 0.17 | | | | 0.03 | [61] |
| 1876 | CCCCCCC | CO | 4.35 | 2.95 | 3.14 | 4.31 | 4.18 | 0.84 | 11.36 | 5.27 | 4.30 | [61] |
| 1877 | CCCCCCC | CCO | 4.24 | 3.27 | 3.20 | 3.88 | 3.76 | 1.07 | 6.91 | 4.40 | 3.90 | [61] |
| 1878 | CCCCCCC | CCCO | 4.17 | 3.07 | 3.01 | 3.72 | 3.56 | 1.17 | 4.69 | 4.10 | 3.71 | [63] |
| 1879 | CCCCCCC | CCCCO | 3.86 | 2.90 | 2.84 | 3.59 | 3.42 | 1.23 | 3.35 | 3.89 | 3.61 | [63] |
| 1880 | CCCCCCC | CCOC(=O)C | 1.29 | 1.10 | 1.12 | 1.23 | 1.37 | 0.14 | 0.29 | 1.64 | 1.17 | [61] |
| 1881 | CCCCCCC | CCCCOC(=O)C | 1.03 | 0.89 | 0.89 | 1.01 | 1.11 | 0.22 | 0.04 | 0.88 | 1.02 | [61] |
| 1882 | CCCCCCC | C1COCCO1 | 1.16 | 1.93 | 1.70 | 1.12 | 1.07 | 0.22 | 1.21 | 1.42 | 1.34 | [61] |
| 1883 | CCCCCCC | CCOC(C)(C)C | 0.31 | 0.22 | 0.20 | 0.14 | | | | | 0.19 | [132] |
| 1884 | CCCCCCC | CC(C)=O | 2.08 | 1.78 | 1.86 | 1.77 | 1.91 | 0.27 | 0.84 | 1.84 | 1.91 | [94] |
| 1885 | CCCCCCC | CCC(C)=O | 1.70 | 1.64 | 1.68 | 1.64 | 1.50 | 0.24 | 0.48 | 1.40 | 1.51 | [61 , 78] |
| 1886 | CCCCCCC | O=C1CCC1 | 1.73 | 1.14 | 1.16 | 1.53 | | 0.43 | 2.37 | | 2.00 | [71] |
| 1887 | CCCCCCC | CC(=O)C(C)=O | 1.79 | 4.94 | 4.97 | 5.23 | | 0.03 | 0.03 | | 2.25 | [71] |
| 1888 | CCCCCCC | CC(=O)CCC(C)=O | 3.50 | 4.23 | 4.23 | 4.57 | | | | | 3.52 | [71] |
| 1889 | CCCCCCC | CCCCl | 0.51 | 0.10 | 0.17 | 0.28 | 0.38 | | | | 0.38 | [61] |
| 1890 | CCCCCCC | CC(C)(C)Cl | 0.66 | 0.02 | 0.04 | 0.04 | 0.31 | | | | 0.36 | [61] |
| 1891 | CCCCCCC | ClCCl | 0.68 | 0.31 | 0.44 | 0.66 | 0.62 | -0.06 | 0.93 | 0.71 | 0.77 | [61] |
| 1892 | CCCCCCC | ClC(Cl)Cl | 0.34 | 0.34 | 0.41 | 0.41 | 0.40 | -0.07 | | 0.43 | 0.38 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1893 | CCCCCCC | ClC(Cl)(Cl)Cl | 0.22 | 0.07 | 0.10 | 0.16 | 0.17 | -0.17 | 0.06 | 0.12 | 0.18 | [61] |
| 1894 | CCCCCCC | CCBr | 0.85 | 0.52 | 0.63 | 0.41 | 0.31 | -0.06 | | | 0.48 | [61] |
| 1895 | CCCCCCC | CC#N | 3.79 | 3.24 | 3.40 | 3.43 | 2.79 | 0.55 | 4.30 | 3.16 | 3.57 | [98] |
| 1896 | CCCCCCC | CCC#N | 2.95 | 2.16 | 2.25 | 2.34 | 2.65 | 0.53 | 1.93 | 2.64 | 3.03 | [61] |
| 1897 | CCCCCCC | CCCC#N | 2.55 | 2.01 | 2.05 | 2.23 | | 0.60 | 1.18 | 2.16 | 2.50 | [98] |
| 1898 | CCCCCCC | C[N+]([O-])=O | 3.51 | 3.63 | 3.77 | 3.02 | 3.38 | 0.65 | 5.07 | 3.42 | 3.65 | [61] |
| 1899 | CCCCCCC | CC[N+]([O-])=O | 2.86 | 2.60 | 2.67 | 2.04 | | 0.69 | 2.82 | | 2.93 | [61] |
| 1900 | CCCCCCC | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 3.76 | 1.60 | 1.57 | 3.07 | | 0.32 | 0.36 | | 3.43 | [63] |
| 1901 | CCCCCCC | CCI | 0.89 | 0.60 | 0.68 | 0.66 | 0.62 | | | | 0.63 | [61] |
| 1902 | CCCCCCC | CCCCN | 1.23 | 0.87 | 0.96 | 1.32 | | 0.21 | 0.34 | | 0.24 | [175] |
| 1903 | CCCCCCC | C(=S)=S | 0.41 | 0.22 | 0.38 | 0.33 | | -0.13 | 1.08 | | 0.25 | [61] |
| 1904 | CCCCCCC | CCSC | 0.59 | 0.48 | 0.52 | 0.54 | | | | | 0.40 | [133 , 134] |
| 1905 | CCCCCCC | CCSCC | 0.61 | 0.26 | 0.29 | 0.25 | | | | | 0.44 | [133 , 134] |
| 1906 | CCCCCCC | CCCSCCC | 0.46 | 0.24 | 0.23 | 0.28 | | | | | 0.31 | [133 , 134] |
| 1907 | CCCCCCC | CSSC | 1.00 | | | 1.12 | | | | | 0.74 | [133 , 134] |
| 1908 | CCCCCCC | CCSSCC | 0.84 | 0.98 | 0.98 | 0.56 | | | | | 0.74 | [133 , 134] |
| 1909 | CCCCCCC | CCCSSCCC | 0.69 | 0.79 | 0.78 | 0.26 | | | | | 0.69 | [133 , 134] |
| 1910 | CCCCCCCO | CCCCC | 0.80 | 0.63 | 0.67 | 0.95 | 1.04 | 0.96 | 1.82 | | 1.07 | [166 , 117] |
| 1911 | CCCCCCCO | CCCCCC | 0.93 | 0.80 | 0.80 | 1.05 | 1.17 | 1.13 | 1.59 | | 1.13 | [166 , 117] |
| 1912 | CCCCCCCO | C1CCCC1 | 0.66 | 0.52 | 0.51 | 0.75 | 0.85 | 0.41 | 0.60 | | 0.80 | [117] |
| 1913 | CCCCCCCO | C1CCCCC1 | 0.78 | 0.72 | 0.66 | 0.94 | 1.01 | 0.79 | 0.52 | | 0.92 | [117] |
| 1914 | CCCCCCCO | CC1CCCC1 | 0.79 | 0.72 | 0.66 | 0.79 | 0.93 | | | | 0.94 | [117] |
| 1915 | CCCCCCCO | c1ccccc1 | 0.62 | 0.58 | 0.49 | 0.77 | 0.75 | 0.44 | -0.11 | | 0.75 | [117] |
| 1916 | CCCCCCCCCCCCCCCC | CCCCC | -0.16 | -0.40 | -0.21 | -0.14 | -0.16 | -0.46 | -0.16 | -0.20 | -0.18 | [176 , 54 , 61 , 61 , 61 , 61 , 171] |
| 1917 | CCCCCCCCCCCCCCCC | CCC(C)C | -0.16 | -0.40 | -0.21 | -0.14 | | -0.34 | 0.26 | | -0.12 | [176 , 61] |
| 1918 | CCCCCCCCCCCCCCCC | CCCCCC | -0.12 | -0.30 | -0.15 | -0.11 | -0.12 | -0.43 | -0.25 | -0.19 | -0.11 | [59 , 176 , 177 , 54 , 61 , 61 , 61 , 61 , 171 , 171 , 178] |
| 1919 | CCCCCCCCCCCCCCCC | C1CCCCC1 | -0.17 | -0.37 | -0.19 | -0.14 | -0.34 | -0.58 | -0.54 | -0.37 | -0.25 | [177 , 54 , 61 , 61 , 61 , 128 , 128 , 128 , 179 , 180 , 181] |
| 1920 | CCCCCCCCCCCCCCCC | CCCC(C)C | -0.13 | -0.30 | -0.15 | -0.11 | -0.06 | | | -0.11 | -0.11 | [176 , 54 , 61 , 61] |
| 1921 | CCCCCCCCCCCCCCCC | CCC(C)CC | -0.13 | -0.30 | -0.15 | -0.11 | -0.13 | | | | -0.17 | [176 , 61] |
| 1922 | CCCCCCCCCCCCCCCC | CC(C)C(C)C | -0.13 | -0.30 | -0.15 | -0.11 | -0.15 | | | -0.09 | -0.16 | [176 , 61] |
| 1923 | CCCCCCCCCCCCCCCC | CCC(C)(C)C | -0.13 | -0.29 | -0.15 | -0.12 | -0.13 | | | | -0.09 | [176 , 61] |
| 1924 | CCCCCCCCCCCCCCCC | CCCCCCC | -0.09 | -0.22 | -0.12 | -0.08 | -0.06 | -0.40 | -0.31 | -0.16 | -0.08 | [176 , 177 , 54 , 61 , 61 , 61 , 61 , 171 , 171] |
| 1925 | CCCCCCCCCCCCCCCC | CCCCCCCC | -0.07 | -0.16 | -0.08 | -0.06 | 0.02 | -0.36 | -0.31 | -0.13 | -0.05 | [176 , 54 , 61 , 61 , 61 , 61 , 171 , 178] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1926 | CCCCCCCCCCCCCCCC | c1ccccc1 | 0.26 | -0.09 | 0.13 | 0.07 | 0.08 | -0.58 | -0.12 | 0.00 | 0.07 | [177 , 177 , 61 , 61 , 182 , 183] |
| 1927 | CCCCCCCCCCCCCCCC | C1CCCC1 | -0.21 | -0.49 | -0.25 | -0.22 | -0.42 | -0.63 | -0.65 | -0.46 | -0.34 | [61] |
| 1928 | CCCCCCCCCCCCCCCC | CC(C)CC(C)C | -0.09 | -0.22 | -0.12 | -0.08 | 0.00 | | | 0.01 | -0.04 | [54 , 61 , 61] |
| 1929 | CCCCCCCCCCCCCCCC | CC(C)CC(C)(C)C | -0.06 | -0.15 | -0.08 | -0.06 | 0.01 | -0.19 | 0.19 | 0.13 | -0.03 | [61] |
| 1930 | CCCCCCCCCCCCCCCC | CC(C)C(C)C(C)C | -0.07 | -0.16 | -0.08 | -0.06 | -0.25 | | | | -0.10 | [61 , 61 , 61] |
| 1931 | CCCCCCCCCCCCCCCC | CC(C)CCC(C)C | -0.06 | -0.16 | -0.08 | -0.06 | | | | | 0.02 | [61] |
| 1932 | CCCCCCCCCCCCCCCC | CCC1CCCCC1 | -0.09 | -0.21 | -0.11 | -0.09 | | | | -0.22 | -0.19 | [61 , 61 , 61] |
| 1933 | CCCCCCCCCCCCCCCC | CCCCCCCCC | -0.05 | -0.12 | -0.06 | -0.05 | 0.19 | -0.34 | -0.31 | -0.11 | -0.02 | [54 , 61 , 61] |
| 1934 | CCCCCCCCCCCCCCCC | CCC(C)CCC(C)C | -0.05 | -0.12 | -0.06 | -0.05 | | | | | -0.07 | [61] |
| 1935 | CCCCCCCCCCCCCCCC | Cc1ccccc1 | 0.30 | 0.03 | 0.17 | 0.05 | 0.04 | -0.48 | -0.17 | 0.02 | -0.02 | [61 , 61] |
| 1936 | CCCCCCCCCCCCCCCC | Cc1cccc(C)c1 | 0.25 | 0.08 | 0.17 | 0.04 | 0.09 | -0.37 | -0.13 | | 0.05 | [61] |
| 1937 | CCCCCCCCCCCCCCCC | Cc1ccc(C)cc1 | 0.25 | 0.08 | 0.17 | 0.04 | 0.03 | -0.39 | -0.21 | 0.00 | 0.01 | [61] |
| 1938 | CCCCCCCCCCCCCCCC | Cc1ccccc1C | 0.29 | 0.08 | 0.17 | 0.04 | 0.10 | -0.39 | -0.14 | | 0.10 | [61] |
| 1939 | CCCCCCCCCCCCCCCC | CCc1ccccc1 | 0.32 | 0.05 | 0.15 | 0.06 | 0.10 | -0.43 | -0.22 | 0.07 | 0.13 | [61] |
| 1940 | CCCCCCCCCCCCCCCC | Cc1cc(C)cc(C)c1 | 0.12 | 0.09 | 0.13 | 0.03 | 0.18 | | | | 0.02 | [61] |
| 1941 | CCCCCCCCCCCCCCCC | CCCC=C | -0.13 | -0.36 | -0.15 | -0.17 | -0.12 | -0.31 | -0.19 | -0.27 | -0.06 | [61 , 61] |
| 1942 | CCCCCCCCCCCCCCCC | CCCCC=C | -0.09 | -0.26 | -0.09 | -0.13 | -0.08 | -0.42 | -0.21 | -0.25 | -0.05 | [61 , 61] |
| 1943 | CCCCCCCCCCCCCCCC | CCCCCC=C | -0.07 | -0.19 | -0.06 | -0.09 | -0.12 | -0.33 | -0.33 | | -0.04 | [61 , 61 , 61] |
| 1944 | CCCCCCCCCCCCCCCC | CCCCCCC=C | -0.04 | -0.13 | -0.04 | -0.06 | -0.02 | -0.31 | -0.34 | -0.15 | -0.06 | [61] |
| 1945 | CCCCCCCCCCCCCCCC | CCCCCCCC=C | -0.03 | -0.08 | -0.02 | -0.04 | | | | | 0.17 | [61] |
| 1946 | CCCCCCCCCCCCCCCC | CO | 4.16 | 2.36 | 2.80 | 3.80 | 3.98 | 0.37 | 19.78 | 5.24 | 4.09 | [61] |
| 1947 | CCCCCCCCCCCCCCCC | CCO | 4.00 | 2.83 | 2.94 | 3.41 | 3.54 | 0.64 | 11.43 | 3.84 | 3.55 | [61 , 61] |
| 1948 | CCCCCCCCCCCCCCCC | CCCO | 3.95 | 2.70 | 2.79 | 3.28 | 3.33 | 0.78 | 7.37 | 3.66 | 3.19 | [61] |
| 1949 | CCCCCCCCCCCCCCCC | CC(C)O | 3.50 | 2.70 | 2.79 | 3.07 | 3.19 | 0.64 | 5.50 | 3.44 | 3.10 | [61] |
| 1950 | CCCCCCCCCCCCCCCC | CCCCO | 3.67 | 2.59 | 2.66 | 3.18 | 3.17 | 0.89 | 4.97 | 3.58 | 3.15 | [61] |
| 1951 | CCCCCCCCCCCCCCCC | CCC(C)O | 3.19 | 2.59 | 2.66 | 2.98 | 2.87 | 0.68 | 3.44 | 3.13 | 2.82 | [61] |
| 1952 | CCCCCCCCCCCCCCCC | CC(C)CO | 3.40 | 2.59 | 2.66 | 3.18 | 3.16 | 0.96 | 4.12 | 3.47 | 3.24 | [61] |
| 1953 | CCCCCCCCCCCCCCCC | CC(C)(C)O | 3.32 | 2.43 | 2.42 | 2.63 | | 0.77 | 2.87 | 2.88 | 2.67 | [61] |
| 1954 | CCCCCCCCCCCCCCCC | CCCCCO | 3.77 | 2.50 | 2.54 | 3.09 | 3.14 | 0.92 | 3.18 | 3.56 | 3.12 | [61] |
| 1955 | CCCCCCCCCCCCCCCC | CC(C)CCO | 3.56 | 2.50 | 2.54 | 3.09 | | 0.77 | 2.38 | | 3.26 | [61] |
| 1956 | CCCCCCCCCCCCCCCC | CCCCCCO | 3.38 | 2.41 | 2.44 | 3.01 | 3.15 | 0.94 | 2.16 | 3.82 | 2.94 | [61] |
| 1957 | CCCCCCCCCCCCCCCC | CCCCCCCCO | 3.26 | 2.26 | 2.26 | 2.87 | 2.93 | 1.19 | 1.75 | 2.85 | 3.01 | [61] |
| 1958 | CCCCCCCCCCCCCCCC | Oc1ccccc1 | 3.40 | 2.42 | 2.60 | 2.90 | 3.43 | 0.75 | 6.53 | 5.60 | 3.07 | [61] |
| 1959 | CCCCCCCCCCCCCCCC | Cc1cccc(O)c1 | 3.20 | 2.29 | 2.41 | 2.72 | | 0.69 | 4.30 | 3.09 | 3.04 | [61] |
| 1960 | CCCCCCCCCCCCCCCC | CC(=O)OC | 1.27 | 0.79 | 1.03 | 1.15 | 1.28 | -0.21 | -0.07 | 1.38 | 0.54 | [61 , 119 , 119] |
| 1961 | CCCCCCCCCCCCCCCC | CCC(=O)OC | 1.02 | 0.72 | 0.91 | 1.02 | 1.00 | -0.04 | | | -0.07 | [119] |
| 1962 | CCCCCCCCCCCCCCCC | CCCC(=O)OC | 0.90 | 0.68 | 0.82 | 0.92 | 0.93 | | | | -0.22 | [119] |
| 1963 | CCCCCCCCCCCCCCCC | CCCCC(=O)OC | 0.82 | 0.64 | 0.76 | 0.85 | | | | | -0.26 | [119] |
| 1964 | CCCCCCCCCCCCCCCC | CCCCCC(=O)OC | 0.77 | 0.62 | 0.70 | 0.79 | 0.81 | | | | -0.49 | [119] |
| 1965 | CCCCCCCCCCCCCCCC | CCOC(=O)C | 1.06 | 0.72 | 0.91 | 1.02 | 1.18 | -0.21 | -0.07 | 1.38 | 0.38 | [61 , 119 , 119] |
| 1966 | CCCCCCCCCCCCCCCC | CCCC(=O)OCC | 0.79 | 0.36 | 0.55 | 0.66 | | -0.01 | | | -0.58 | [119] |
| 1967 | CCCCCCCCCCCCCCCC | CCCOC(=O)C | 0.92 | 0.68 | 0.82 | 0.92 | -3.00 | 0.01 | -0.34 | 1.21 | 0.41 | [61 , 119] |
| 1968 | CCCCCCCCCCCCCCCC | CCCCOC(=O)C | 0.85 | 0.64 | 0.76 | 0.85 | 0.89 | -0.05 | -0.34 | 0.67 | 0.31 | [61 , 119] |
| 1969 | CCCCCCCCCCCCCCCC | CCCCCOC(=O)C | 0.78 | 0.62 | 0.70 | 0.79 | | | | | -0.24 | [119] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1970 | CCCCCCCCCCCCCCCC | C1CCOC1 | 0.27 | 0.10 | 0.26 | 0.07 | -0.11 | -0.27 | 0.44 | 0.05 | 0.17 | [61] |
| 1971 | CCCCCCCCCCCCCCCC | C1COCCO1 | 0.94 | 1.58 | 1.47 | 0.82 | 0.77 | -0.27 | 1.35 | 0.95 | 0.88 | [61] |
| 1972 | CCCCCCCCCCCCCCCC | CCOCC | 0.10 | -0.19 | 0.03 | 0.02 | 0.20 | -0.30 | -0.54 | 0.11 | 0.03 | [61] |
| 1973 | CCCCCCCCCCCCCCCC | COc1ccccc1 | 0.95 | 1.02 | 1.17 | 0.84 |  | -0.11 | 0.60 | 0.84 | 0.76 | [61] |
| 1974 | CCCCCCCCCCCCCCCC | CCC(C)=O | 1.44 | 1.23 | 1.45 | 1.29 | 1.29 | -0.11 | 0.21 | 1.11 | 1.23 | [61 , 61] |
| 1975 | CCCCCCCCCCCCCCCC | CCCC(C)=O | 1.25 | 1.17 | 1.34 | 1.21 | 1.13 | -0.07 | -0.11 | 0.91 | 1.15 | [61] |
| 1976 | CCCCCCCCCCCCCCCC | CC(=O)c1ccccc1 | 1.91 | 2.18 | 2.29 | 2.46 | 1.51 | 0.39 | 2.95 | 1.10 | 1.73 | [61] |
| 1977 | CCCCCCCCCCCCCCCC | CCC=O | 1.29 | 1.00 | 1.29 | 1.05 |  |  |  |  | 1.12 | [61] |
| 1978 | CCCCCCCCCCCCCCCC | CCCC=O | 1.09 | 0.96 | 1.18 | 0.99 | 1.12 | -0.22 | -0.62 | 0.77 | 1.06 | [61] |
| 1979 | CCCCCCCCCCCCCCCC | CCCCl | 0.27 | -0.33 | -0.07 | 0.07 | 0.15 |  |  |  | 0.15 | [61] |
| 1980 | CCCCCCCCCCCCCCCC | CCCCCl | 0.26 | -0.24 | -0.03 | 0.07 | 0.17 | -0.39 | -0.45 | 0.09 | 0.19 | [61 , 61] |
| 1981 | CCCCCCCCCCCCCCCC | CC(C)(C)Cl | 0.44 | -0.34 | -0.16 | -0.14 | 0.10 |  |  |  | 0.27 | [61] |
| 1982 | CCCCCCCCCCCCCCCC | ClCCl | 0.39 | -0.21 | 0.16 | 0.38 | 0.34 | -0.54 | 0.91 | 0.25 | 0.36 | [61 , 61] |
| 1983 | CCCCCCCCCCCCCCCC | ClC(Cl)Cl | 0.06 | -0.14 | 0.17 | 0.04 | 0.08 | -0.51 |  | 0.05 | 0.08 | [61 , 61] |
| 1984 | CCCCCCCCCCCCCCCC | ClC(Cl)(Cl)Cl | -0.05 | -0.34 | -0.11 | -0.17 | -0.17 | -0.58 | -0.37 | -0.29 | -0.19 | [61] |
| 1985 | CCCCCCCCCCCCCCCC | Clc1ccccc1 | 0.40 | 0.16 | 0.29 | 0.05 | 0.15 | -0.30 | 0.66 | 0.06 | 0.22 | [61] |
| 1986 | CCCCCCCCCCCCCCCC | CCBr | 0.62 | 0.03 | 0.36 | 0.13 | 0.03 | -0.46 |  |  | 0.25 | [61] |
| 1987 | CCCCCCCCCCCCCCCC | CC#N | 3.42 | 2.68 | 3.09 | 2.87 | 2.56 | 0.12 | 6.74 | 2.49 | 2.98 | [61] |
| 1988 | CCCCCCCCCCCCCCCC | CCC#N | 2.61 | 1.67 | 1.99 | 1.82 | 2.44 | 0.16 | 2.55 | 2.19 | 2.54 | [61] |
| 1989 | CCCCCCCCCCCCCCCC | CCCC#N | 2.24 | 1.59 | 1.83 | 1.74 |  | 0.27 | 1.29 | 1.83 | 2.26 | [61] |
| 1990 | CCCCCCCCCCCCCCCC | C[N+](=O)[O-] | 3.17 | 3.09 | 3.46 | 2.44 | 3.13 | 0.22 | 8.13 | 2.82 | 3.10 | [61] |
| 1991 | CCCCCCCCCCCCCCCC | CC[N+](=O)[O-] | 2.55 | 2.13 | 2.41 | 1.59 |  | 0.29 | 4.07 |  | 2.57 | [61] |
| 1992 | CCCCCCCCCCCCCCCC | CC(C)[N+](=O)[O-] | 1.85 | 1.33 | 1.55 | 1.44 |  | 0.20 | 1.54 |  | 2.30 | [61] |
| 1993 | CCCCCCCCCCCCCCCC | CCI | 0.66 | 0.12 | 0.43 | 0.25 | 0.21 |  |  |  | 0.22 | [61] |
| 1994 | CCCCCCCCCCCCCCCC | CCNCC | 0.47 | -0.06 | 0.15 | 0.11 | 0.12 | -0.29 | -0.60 |  | 0.10 | [61] |
| 1995 | CCCCCCCCCCCCCCCC | CCCNCCC | 0.44 | 0.04 | 0.16 | 0.17 |  | -0.27 |  |  | 0.11 | [61] |
| 1996 | CCCCCCCCCCCCCCCC | CCN(CC)CC | 0.03 | -0.19 | -0.07 | -0.03 | 0.00 | -0.37 | -0.17 | -0.03 | -0.07 | [61] |
| 1997 | CCCCCC | c1ccccc1 | 0.56 | 0.45 | 0.38 | 0.55 | 0.53 | -0.02 | 0.38 | 0.51 | 0.52 | [184 , 184 , 78 , 109 , 106 , 106 , 107] |
| 1998 | CCCCCC | CCCCC | 0.00 | -0.01 | -0.01 | 0.00 | 0.15 | -0.22 | -0.22 | -0.01 | -0.04 | [54 , 61] |
| 1999 | CCCCCC | C1CCCCC1 | 0.01 | 0.03 | 0.00 | 0.10 | 0.10 | -0.15 | -0.05 | 0.11 | 0.12 | [54 , 61 , 128 , 128] |
| 2000 | CCCCCC | CCCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | 0.29 |  |  | 0.02 | -0.03 | [54 , 61] |
| 2001 | CCCCCC | CCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.35 | -0.16 | -0.16 | 0.02 | -0.01 | [54 , 61] |
| 2002 | CCCCCC | CC(C)CC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | 0.38 |  |  | 0.03 | -0.12 | [54] |
| 2003 | CCCCCC | CCCCCCCC | -0.01 | -0.03 | -0.02 | 0.00 | 0.49 | -0.13 | -0.13 | 0.02 | 0.06 | [54 , 61 , 61 , 178] |
| 2004 | CCCCCC | CC(C)C(C)C(C)C | -0.01 | -0.03 | -0.02 | 0.00 | 0.20 |  |  |  | 0.07 | [54 , 61] |
| 2005 | CCCCCC | CC(C)CCC(C)C | -0.01 | -0.03 | -0.02 | 0.00 |  |  |  |  | 0.07 | [54] |
| 2006 | CCCCCC | CCC1CCCCC1 | 0.01 | 0.04 | -0.01 | 0.10 |  |  |  | 0.13 | 0.16 | [54 , 61] |
| 2007 | CCCCCC | CCCCCCCCC | -0.03 | -0.07 | -0.03 | -0.01 | 0.71 | -0.09 | -0.09 | 0.02 | 0.08 | [54 , 61] |
| 2008 | CCCCCC | CCC(C)CCC(C)C | -0.03 | -0.07 | -0.03 | -0.01 |  |  |  |  | 0.03 | [61] |
| 2009 | CCCCCC | Cc1ccccc1 | 0.56 | 0.48 | 0.37 | 0.55 | 0.55 | 0.04 | 0.31 | 0.49 | 0.50 | [61 , 78] |
| 2010 | CCCCCC | CCO | 4.27 | 3.32 | 3.24 | 3.97 | 3.82 | 1.13 | 6.64 | 4.45 | 4.01 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2011 | CCCCCC | CCCO | 4.20 | 3.10 | 3.03 | 3.81 | 3.66 | 1.23 | 4.58 | 4.15 | 3.78 | [63 , 61] |
| 2012 | CCCCCC | CC(C)O | 3.74 | 3.10 | 3.03 | 3.53 | 3.49 | 1.07 | 3.60 | 3.82 | 3.44 | [61] |
| 2013 | CCCCCC | CCCCO | 3.88 | 2.91 | 2.85 | 3.68 | 3.56 | 1.29 | 3.33 | 3.93 | 3.59 | [61] |
| 2014 | CCCCCC | CCOC(=O)C | 1.32 | 1.13 | 1.14 | 1.26 | 1.52 | 0.19 | 0.41 | 1.66 | 1.23 | [61 , 124] |
| 2015 | CCCCCC | CCCOC(=O)C | 1.15 | 1.00 | 1.00 | 1.13 | -2.53 | 0.31 | 0.17 | 1.35 | 0.24 | [119] |
| 2016 | CCCCCC | C1CCOC1 | 0.54 | 0.49 | 0.48 | 0.36 | 0.29 | 0.20 | 0.76 | 0.51 | 0.52 | [61] |
| 2017 | CCCCCC | C1COCCO1 | 1.18 | 1.95 | 1.72 | 1.18 | 1.20 | 0.32 | 1.31 | 1.50 | 1.39 | [61] |
| 2018 | CCCCCC | CCOC(C)(C)C | 0.31 | 0.21 | 0.21 | 0.14 | | | | | 0.16 | [132] |
| 2019 | CCCCCC | CC(C)=O | 2.13 | 1.84 | 1.89 | 1.84 | 2.00 | 0.32 | 0.96 | 1.86 | 1.90 | [94] |
| 2020 | CCCCCC | CCC(C)=O | 1.74 | 1.68 | 1.70 | 1.71 | 1.64 | 0.30 | 0.60 | 1.44 | 1.49 | [61 , 124] |
| 2021 | CCCCCC | CCCCCl | 0.51 | 0.17 | 0.17 | 0.26 | 0.56 | 0.02 | 0.08 | 0.44 | 0.43 | [61] |
| 2022 | CCCCCC | CC(C)(C)Cl | 0.68 | 0.05 | 0.05 | 0.06 | 0.45 | | | | 0.39 | [61] |
| 2023 | CCCCCC | ClCCCl | 1.00 | 0.89 | 0.94 | 1.17 | 1.17 | 0.31 | 1.48 | 1.23 | 1.15 | [124] |
| 2024 | CCCCCC | ClC(Cl)Cl | 0.39 | 0.39 | 0.44 | 0.48 | 0.48 | 0.02 | | 0.49 | 0.48 | [61] |
| 2025 | CCCCCC | ClC(Cl)(Cl)Cl | 0.26 | 0.10 | 0.12 | 0.21 | 0.26 | -0.08 | 0.17 | 0.20 | 0.17 | [61] |
| 2026 | CCCCCC | CCBr | 0.89 | 0.59 | 0.66 | 0.45 | 0.39 | 0.01 | | | 0.52 | [61] |
| 2027 | CCCCCC | CCC#N | 3.01 | 2.22 | 2.29 | 2.45 | 2.77 | 0.59 | 2.00 | 2.70 | 2.92 | [61] |
| 2028 | CCCCCC | CCCC#N | 2.61 | 2.05 | 2.08 | 2.33 | | 0.65 | 1.28 | 2.21 | 2.36 | [98] |
| 2029 | CCCCCC | CC[N+]([O-])=O | 2.92 | 2.65 | 2.70 | 2.13 | | 0.75 | 2.83 | | 3.02 | [61 , 124 , 66] |
| 2030 | CCCCCC | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | 3.32 | 1.42 | 1.40 | 2.83 | | | | | 2.89 | [63] |
| 2031 | CCCCCC | CCI | 0.93 | 0.66 | 0.71 | 0.74 | 0.65 | | | | 0.73 | [124] |
| 2032 | CCCCCC | CCN(CC)CC | 0.14 | 0.05 | 0.05 | 0.07 | 0.41 | 0.11 | 0.28 | 0.08 | 0.10 | [61 , 124] |
| 2033 | CCCCCCCCCCCCCCCCI | Cc1cccc(C)c1 | | -0.25 | -0.11 | -0.34 | | | | | -0.25 | [61] |
| 2034 | CCCCCCCCCCCCCCCCI | Cc1ccc(C)cc1 | | -0.25 | -0.11 | -0.34 | | | | | -0.27 | [61] |
| 2035 | CCCCCCCCCCCCCCCCI | Cc1ccccc1C | | -0.25 | -0.11 | -0.34 | | | | | -0.26 | [61] |
| 2036 | CCCCCCCCCCCCCCCCI | CCc1ccccc1 | | -0.25 | -0.09 | -0.24 | | | | | -0.20 | [61] |
| 2037 | CCCCCCCCCCCCCCCCI | CCCc1ccccc1 | | -0.19 | -0.07 | -0.20 | | | | | -0.15 | [61] |
| 2038 | CCCCCCCCCCCCCCCCI | Cc1cc(C)cc(C)c1 | | -0.22 | -0.13 | -0.37 | | | | | -0.22 | [61] |
| 2039 | CCCCCCCCCCCCCCCCI | CC(C)c1ccccc1 | | -0.21 | -0.09 | -0.20 | | | | | -0.12 | [61] |
| 2040 | [O-][N+](=O)c1ccccc1 | CCCCCC | 2.08 | 2.07 | 1.95 | 2.35 | 2.16 | 1.40 | 1.15 | 2.04 | 2.02 | [59 , 59 , 73 , 54 , 61 , 61 , 47] |
| 2041 | [O-][N+](=O)c1ccccc1 | c1ccccc1 | 0.34 | 0.39 | 0.40 | 0.20 | 0.06 | 0.25 | -0.06 | 0.26 | 0.28 | [59 , 59 , 73 , 47 , 61 , 47] |
| 2042 | [O-][N+](=O)c1ccccc1 | CCCCC | 1.83 | 1.81 | 1.68 | 2.17 | 2.01 | 1.31 | 1.32 | 1.88 | 1.86 | [54 , 61 , 61] |
| 2043 | [O-][N+](=O)c1ccccc1 | C1CCCCC1 | 1.68 | 1.66 | 1.64 | 2.00 | 1.52 | 0.67 | 0.39 | 1.66 | 1.76 | [54 , 61 , 61 , 47] |
| 2044 | [O-][N+](=O)c1ccccc1 | CCCC(C)C | 2.02 | 2.07 | 1.94 | 2.35 | 2.17 | | | 2.13 | 2.07 | [54 , 61 , 61] |
| 2045 | [O-][N+](=O)c1ccccc1 | CCCCCCC | 2.31 | 2.32 | 2.21 | 2.54 | 2.30 | 1.47 | 1.00 | 2.22 | 2.20 | [54 , 61 , 61] |
| 2046 | [O-][N+](=O)c1ccccc1 | CC(C)CC(C)C | 2.18 | 2.31 | 2.20 | 2.54 | 2.30 | | | 2.40 | 2.26 | [54 , 61 , 61] |
| 2047 | [O-][N+](=O)c1ccccc1 | CC1CCCCC1 | 1.90 | 1.92 | 1.90 | 2.11 | 1.68 | 0.99 | 0.68 | 1.93 | 1.94 | [61] |
| 2048 | [O-][N+](=O)c1ccccc1 | CCCCCCCC | 2.54 | 2.55 | 2.46 | 2.73 | 2.50 | 1.59 | 0.93 | 2.40 | 2.32 | [54 , 61 , 61 , 61] |
| 2049 | [O-][N+](=O)c1ccccc1 | CC(C)CC(C)(C)C | 2.34 | 2.62 | 2.50 | 2.73 | 2.37 | 2.20 | 1.59 | 2.67 | 2.42 | [61] |
| 2050 | [O-][N+](=O)c1ccccc1 | CC(C)C(C)C(C)C | 2.27 | 2.54 | 2.46 | 2.73 | 2.19 | | | | 2.26 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2051 | [O-][N+](=O)c1ccccc1 | CC(C)CCC(C)C | 2.45 | 2.54 | 2.46 | 2.73 | | | | | 2.48 | [61] |
| 2052 | [O-][N+](=O)c1ccccc1 | CCC1CCCCC1 | 2.11 | 2.16 | 2.16 | 2.32 | | | | 2.15 | 2.05 | [54 , 61 , 61] |
| 2053 | [O-][N+](=O)c1ccccc1 | CCCCCCCCC | 2.76 | 2.76 | 2.71 | 2.92 | 2.77 | 1.69 | 0.86 | 2.58 | 2.52 | [54 , 61 , 61] |
| 2054 | [O-][N+](=O)c1ccccc1 | CCC(C)CCC(C)C | 2.62 | 2.76 | 2.71 | 2.92 | | | | | 2.33 | [61] |
| 2055 | [O-][N+](=O)c1ccccc1 | Cc1ccccc1 | 0.53 | -0.14 | -0.14 | 0.29 | 0.13 | 0.28 | 0.04 | 0.49 | 0.34 | [61] |
| 2056 | [O-][N+](=O)c1ccccc1 | CCCC=C | 1.19 | 0.52 | 0.41 | 0.66 | 1.63 | 1.15 | 1.32 | 1.37 | 1.48 | [61] |
| 2057 | [O-][N+](=O)c1ccccc1 | CC=C(C)C | 1.15 | 1.14 | 0.94 | 1.20 | | 0.93 | 1.09 | | 1.25 | [47] |
| 2058 | [O-][N+](=O)c1ccccc1 | CC(C)C=C | 1.22 | 0.52 | 0.41 | 0.66 | | | | | 1.29 | [61] |
| 2059 | [O-][N+](=O)c1ccccc1 | CC(=C)C=C | 0.77 | -0.30 | -0.39 | -0.49 | 0.99 | | | | 0.87 | [61 , 47] |
| 2060 | [O-][N+](=O)c1ccccc1 | CO | 2.18 | 2.24 | 2.20 | 1.06 | 2.50 | 0.54 | 2.88 | 2.83 | 2.30 | [61] |
| 2061 | [O-][N+](=O)c1ccccc1 | CCO | 2.25 | 2.29 | 1.89 | 2.50 | 2.41 | 0.70 | 1.12 | 2.44 | 2.21 | [61] |
| 2062 | [O-][N+](=O)c1ccccc1 | CCOC(=O)C | 0.08 | -0.30 | -0.48 | 0.06 | 0.49 | 0.20 | -0.13 | -0.02 | 0.31 | [61] |
| 2063 | [O-][N+](=O)c1ccccc1 | C1COCCO1 | -0.01 | 0.86 | 0.21 | -1.56 | -0.54 | 0.07 | -0.25 | -0.19 | -0.20 | [61] |
| 2064 | [O-][N+](=O)c1ccccc1 | CC(C)=O | 0.01 | 0.26 | 0.14 | 0.46 | 0.43 | 0.12 | -0.27 | -0.14 | 0.22 | [61] |
| 2065 | [O-][N+](=O)c1ccccc1 | CCC(C)=O | 0.05 | 0.36 | 0.22 | 0.51 | 0.22 | 0.12 | -0.14 | -0.13 | 0.04 | [61] |
| 2066 | [O-][N+](=O)c1ccccc1 | CCCCl | 0.35 | 0.52 | 0.43 | 1.05 | 0.62 | | | | 0.58 | [61] |
| 2067 | [O-][N+](=O)c1ccccc1 | CC(C)(C)Cl | 0.46 | 1.23 | 1.07 | 1.52 | 1.06 | | | | 0.86 | [61] |
| 2068 | [O-][N+](=O)c1ccccc1 | ClCCl | -0.34 | -1.08 | -1.11 | -0.87 | -0.16 | -0.25 | -0.34 | -0.26 | -0.01 | [61] |
| 2069 | [O-][N+](=O)c1ccccc1 | ClC(Cl)Cl | -0.22 | -1.11 | -1.14 | -1.27 | -0.14 | -0.01 | | -0.24 | 0.02 | [61] |
| 2070 | [O-][N+](=O)c1ccccc1 | ClC(Cl)(Cl)Cl | 0.86 | 0.82 | 0.73 | 1.08 | 0.53 | 0.41 | 0.10 | 0.82 | 0.80 | [61] |
| 2071 | [O-][N+](=O)c1ccccc1 | CCBr | -0.51 | -0.19 | -0.25 | 0.72 | 0.43 | -0.05 | | | 0.40 | [61] |
| 2072 | [O-][N+](=O)c1ccccc1 | CCI | -0.58 | 0.97 | 0.95 | 0.12 | 0.60 | | | | 0.59 | [61] |
| 2073 | [O-][N+](=O)c1ccccc1 | CCN(CC)CC | 1.40 | 0.84 | 0.73 | 1.58 | 0.97 | 0.68 | 0.17 | 1.44 | 1.38 | [61] |
| 2074 | [O-][N+](=O)c1ccccc1 | C(=S)=S | 0.25 | -0.73 | -0.63 | -0.21 | | -0.04 | -0.36 | | 0.95 | [61] |
| 2075 | CC[N+]([O-])=O | CCCCCCCC | 3.57 | 2.10 | 2.29 | 2.49 | | 2.51 | 1.44 | 3.04 | 3.04 | [61] |
| 2076 | CC[N+]([O-])=O | c1ccccc1 | 0.85 | 0.69 | 0.51 | 0.54 | | 1.31 | 0.36 | 0.71 | 0.59 | [61] |
| 2077 | CC[N+]([O-])=O | Cc1ccccc1 | 1.04 | 1.04 | 0.85 | 0.69 | | 1.31 | 0.49 | 0.94 | 0.73 | [61] |
| 2078 | CC[N+]([O-])=O | CCCC=C | 1.73 | 1.32 | 1.34 | 1.32 | | 1.32 | 1.85 | 1.71 | 1.62 | [61] |
| 2079 | CC[N+]([O-])=O | CC(C)C=C | 1.68 | 1.32 | 1.34 | 1.32 | | | | | 1.58 | [61] |
| 2080 | CC[N+]([O-])=O | CC(=C)C=C | 1.16 | 1.14 | 1.14 | 0.69 | | | | | 0.91 | [61] |
| 2081 | CC[N+]([O-])=O | CO | 1.88 | 1.49 | 1.53 | 1.85 | | 0.43 | 0.98 | 2.11 | 1.77 | [61] |
| 2082 | CC[N+]([O-])=O | CCO | 2.02 | 1.61 | 1.53 | 1.94 | | 0.70 | 0.17 | 1.95 | 1.88 | [61] |
| 2083 | CC[N+]([O-])=O | C1COCCO1 | -0.01 | 0.08 | -0.06 | 0.01 | | 1.04 | -0.01 | 0.28 | -0.13 | [61] |
| 2084 | CC[N+]([O-])=O | CCC(C)=O | -0.01 | -0.12 | -0.12 | -0.33 | | 0.09 | 0.25 | 0.13 | -0.13 | [61] |
| 2085 | CC[N+]([O-])=O | CCCCl | 0.62 | 0.67 | 0.67 | 0.48 | | | | | 0.63 | [61] |
| 2086 | CC[N+]([O-])=O | CC(C)(C)Cl | 0.68 | 1.13 | 1.16 | 1.13 | | | | | 0.83 | [61] |
| 2087 | CC[N+]([O-])=O | ClCCl | -0.26 | 0.17 | 0.17 | -0.03 | | 0.19 | -0.04 | -0.01 | -0.08 | [61] |
| 2088 | CC[N+]([O-])=O | ClC(Cl)Cl | 0.13 | -0.46 | -0.49 | -0.29 | | 0.65 | | 0.08 | 0.00 | [61] |
| 2089 | CC[N+]([O-])=O | ClC(Cl)(Cl)Cl | 1.55 | 1.20 | 1.20 | 1.06 | | 1.45 | 0.57 | 1.39 | 1.35 | [61] |
| 2090 | CC[N+]([O-])=O | CCBr | 0.08 | 0.48 | 0.48 | 0.80 | | 0.07 | | | 0.52 | [61] |
| 2091 | CC[N+]([O-])=O | CCI | 0.19 | 1.08 | 1.05 | 1.05 | | | | | 1.01 | [61] |
| 2092 | CC[N+]([O-])=O | C(=S)=S | 1.43 | 1.80 | 1.76 | 1.96 | | | | | 1.59 | [61] |
| 2093 | C[N+]([O-])=O | CCCCCC | 4.19 | 2.65 | 2.84 | 3.89 | 4.04 | 2.97 | 2.19 | 3.79 | 3.82 | [73 , 54 , 61 , 61 , 61 , 47] |
| 2094 | C[N+]([O-])=O | c1ccccc1 | 1.54 | 1.28 | 1.06 | 1.31 | 1.34 | 2.00 | 0.84 | 1.38 | 1.22 | [73 , 61 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2095 | C[N+]([O-])=O | CCCCC | 3.71 | 2.37 | 2.48 | 3.53 | 3.67 | 2.63 | 2.36 | 3.37 | 3.43 | [54 , 61 , 61] |
| 2096 | C[N+]([O-])=O | C1CCCCC1 | 3.63 | 2.41 | 2.40 | 3.81 | 3.59 | 2.42 | 1.41 | 3.63 | 3.55 | [54 , 61 , 61] |
| 2097 | C[N+]([O-])=O | CCCC(C)C | 4.05 | 2.64 | 2.84 | 3.89 | 3.99 | | | 3.75 | 3.76 | [54 , 61 , 61] |
| 2098 | C[N+]([O-])=O | CCCCCCC | 4.66 | 2.90 | 3.19 | 4.25 | 4.40 | 3.33 | 2.03 | 4.20 | 4.35 | [54 , 61 , 61] |
| 2099 | C[N+]([O-])=O | CC(C)CC(C)C | 4.35 | 2.90 | 3.18 | 4.25 | 4.24 | | | 4.11 | 4.08 | [54 , 61 , 61] |
| 2100 | C[N+]([O-])=O | CCCCCCCC | 5.13 | 3.14 | 3.53 | 4.61 | 4.81 | 3.70 | 1.95 | 4.59 | 4.77 | [54 , 61 , 61 , 61] |
| 2101 | C[N+]([O-])=O | CC(C)C(C)C(C)C | 4.56 | 3.13 | 3.52 | 4.61 | 4.42 | | | | 4.31 | [54 , 61 , 61] |
| 2102 | C[N+]([O-])=O | CC(C)CCC(C)C | 4.86 | 3.13 | 3.53 | 4.61 | | | | | 4.57 | [54] |
| 2103 | C[N+]([O-])=O | CCC1CCCCC1 | 4.46 | 2.93 | 3.10 | 4.31 | | | | 4.44 | 4.31 | [54 , 61 , 61] |
| 2104 | C[N+]([O-])=O | CCCCCCCCC | 5.59 | 3.36 | 3.87 | 4.97 | 5.29 | 4.07 | 1.87 | 5.00 | 5.21 | [54 , 61 , 61] |
| 2105 | C[N+]([O-])=O | Cc1ccccc1 | 1.70 | 1.69 | 1.52 | 1.61 | 1.63 | 2.06 | 0.96 | 1.71 | 1.64 | [61] |
| 2106 | C[N+]([O-])=O | CC(=C)C=C | 1.91 | 1.79 | 1.81 | 1.50 | 2.37 | | | | 1.87 | [61] |
| 2107 | C[N+]([O-])=O | CCCCCC=C | 3.50 | 2.57 | 2.81 | 3.39 | 3.77 | 2.70 | 2.04 | | 3.35 | [61] |
| 2108 | C[N+]([O-])=O | CCO | 2.16 | 1.67 | 1.65 | 2.14 | 2.09 | 0.90 | -0.13 | 2.18 | 2.11 | [61] |
| 2109 | C[N+]([O-])=O | CCC(C)=O | 0.08 | 0.02 | 0.08 | 0.16 | 0.38 | 0.43 | 0.69 | 0.22 | 0.20 | [61] |
| 2110 | C[N+]([O-])=O | CCCCl | 1.23 | 1.36 | 1.39 | 1.50 | 1.56 | | | | 1.47 | [61] |
| 2111 | C[N+]([O-])=O | CC(C)(C)Cl | 1.29 | 1.91 | 2.02 | 2.44 | 2.22 | | | | 1.68 | [61] |
| 2112 | C[N+]([O-])=O | ClCCl | 0.25 | 0.55 | 0.54 | 0.54 | 0.25 | 0.55 | 0.36 | 0.64 | 0.51 | [61] |
| 2113 | C[N+]([O-])=O | ClC(Cl)Cl | 0.92 | -0.01 | -0.03 | 0.33 | 0.59 | 1.16 | | 0.90 | 0.77 | [61] |
| 2114 | C[N+]([O-])=O | ClC(Cl)(Cl)Cl | 2.47 | 1.89 | 1.94 | 2.02 | 2.03 | 2.20 | 1.06 | 2.44 | 2.14 | [61] |
| 2115 | C[N+]([O-])=O | CCBr | 0.42 | 0.87 | 0.87 | 1.86 | 1.47 | 0.41 | | | 1.25 | [61] |
| 2116 | C[N+]([O-])=O | CCI | 0.59 | 1.57 | 1.55 | 1.80 | 2.09 | | | | 1.79 | [61] |
| 2117 | C[N+]([O-])=O | CCN(CC)CC | 2.13 | 2.16 | 2.42 | 3.58 | 2.59 | 3.08 | 1.09 | 2.44 | 2.51 | [61] |
| 2118 | C[N+]([O-])=O | C(=S)=S | 2.15 | 2.87 | 2.77 | 3.57 | | 1.52 | 0.29 | | 2.67 | [61] |
| 2119 | CO | CCCCC | 2.95 | 2.67 | 2.91 | 2.87 | 3.04 | 4.49 | 3.73 | 3.27 | 3.12 | [166 , 54 , 123 , 100] |
| 2120 | CO | CCCCCC | 3.32 | 2.94 | 3.31 | 3.13 | 3.36 | 5.10 | 3.55 | 3.58 | 3.29 | [166 , 73 , 54 , 61 , 61 , 47 , 100 , 174] |
| 2121 | CO | CCCCCCC | 3.68 | 3.20 | 3.72 | 3.39 | 3.66 | 5.73 | 3.36 | 3.90 | 3.63 | [166 , 54 , 61 , 61 , 100 , 174] |
| 2122 | CO | CCCCCCCC | 4.03 | 3.43 | 4.12 | 3.66 | 4.02 | 6.36 | 3.27 | 4.22 | 3.85 | [166 , 54 , 61 , 61 , 61] |
| 2123 | CO | c1ccccc1 | 2.02 | 1.82 | 1.54 | 1.98 | 2.05 | 3.20 | 1.98 | 2.18 | 1.99 | [73 , 61 , 61 , 123 , 47 , 96 , 100] |
| 2124 | CO | C1CCCCC1 | 2.95 | 2.75 | 2.80 | 3.06 | 3.22 | 4.21 | 2.67 | 3.36 | 3.09 | [54 , 61 , 61 , 61] |
| 2125 | CO | CCCC(C)C | 3.20 | 2.94 | 3.31 | 3.13 | 3.32 | | | 3.59 | 3.15 | [54 , 61 , 61] |
| 2126 | CO | CC(C)CC(C)C | 3.41 | 3.19 | 3.71 | 3.39 | 3.54 | | | 3.91 | 3.37 | [54 , 61] |
| 2127 | CO | CC(C)C(C)C(C)C | 3.57 | 3.43 | 4.10 | 3.66 | 3.64 | | | | 3.60 | [54 , 61 , 61] |
| 2128 | CO | CC(C)CCC(C)C | 3.80 | 3.43 | 4.11 | 3.66 | | | | | 3.68 | [54] |
| 2129 | CO | CCC1CCCCC1 | 3.57 | 3.28 | 3.60 | 3.46 | | | | 4.03 | 3.65 | [54 , 61 , 61] |
| 2130 | CO | CCCCCCCCC | 4.38 | 3.66 | 4.51 | 3.93 | 4.45 | 7.01 | 3.18 | 4.54 | 4.16 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2131 | CO | CCC(C)CCC(C)C | 4.11 | 3.66 | 4.51 | 3.93 | | | | | 3.59 | [61] |
| 2132 | CO | Cc1ccccc1 | 2.38 | 2.08 | 1.89 | 2.28 | 2.29 | 3.58 | 2.13 | 2.43 | 2.29 | [61 , 100] |
| 2133 | CO | Cc1cccc(C)c1 | 2.67 | 2.26 | 2.18 | 2.61 | 2.56 | 3.89 | 2.16 | | 2.86 | [100] |
| 2134 | CO | Cc1ccc(C)cc1 | 2.68 | 2.26 | 2.18 | 2.61 | 2.49 | 3.83 | 2.24 | 2.70 | 2.80 | [100] |
| 2135 | CO | Cc1ccccc1C | 2.57 | 2.26 | 2.18 | 2.61 | 2.53 | 3.80 | 2.16 | | 2.83 | [100] |
| 2136 | CO | CCc1ccccc1 | 2.66 | 2.35 | 2.29 | 2.65 | 2.60 | 4.43 | 2.25 | 2.85 | 2.51 | [100] |
| 2137 | CNC=O | CCCCC | 3.63 | | | 3.41 | 3.32 | 4.39 | 5.74 | 3.53 | 3.13 | [54] |
| 2138 | CNC=O | CCCCCC | 4.13 | | | 3.71 | 3.67 | 4.93 | 5.46 | 3.87 | 3.61 | [54] |
| 2139 | CNC=O | C1CCCCC1 | 3.56 | | | 3.05 | 3.34 | 3.85 | 4.15 | 3.36 | 3.15 | [54] |
| 2140 | CNC=O | CCCC(C)C | 3.99 | | | 3.71 | 3.62 | | | 3.95 | 3.54 | [54] |
| 2141 | CNC=O | CCCCCCC | 4.61 | | | 4.02 | 4.02 | 5.48 | 5.19 | 4.23 | 4.02 | [54] |
| 2142 | CNC=O | CC(C)CC(C)C | 4.32 | | | 4.02 | 3.87 | | | 4.37 | 3.88 | [54] |
| 2143 | CNC=O | CCCCCCCC | 5.10 | | | 4.32 | 4.41 | 6.06 | 5.06 | 4.58 | 4.40 | [54] |
| 2144 | CNC=O | CC(C)C(C)C(C)C | 4.54 | | | 4.32 | 4.02 | | | | 4.04 | [54] |
| 2145 | CNC=O | CC(C)CCC(C)C | 4.85 | | | 4.32 | | | | | 4.25 | [54] |
| 2146 | CNC=O | CCC1CCCCC1 | 4.42 | | | 3.54 | | | | 4.19 | 3.82 | [54] |
| 2147 | CNC=O | CCCCCCCCC | 5.57 | | | 4.62 | 4.89 | 6.64 | 4.92 | 4.94 | 4.75 | [54] |
| 2148 | CN1CCCCC1 | C1CCCCC1 | 0.09 | 1.20 | 1.20 | 1.55 | | | | | 0.05 | [160] |
| 2149 | CN1CCCC1=O | CCCCCC | 2.06 | 2.22 | 2.19 | 2.33 | 2.67 | 1.78 | 2.48 | 2.68 | 2.66 | [59 , 147 , 54 , 47] |
| 2150 | CN1CCCC1=O | c1ccccc1 | 0.08 | 0.04 | 0.03 | -0.09 | 0.31 | 0.75 | 0.60 | 0.10 | 0.02 | [59 , 59 , 47 , 73 , 164] |
| 2151 | CN1CCCC1=O | CCCCC | 1.79 | 1.93 | 1.89 | 2.11 | 2.36 | 1.61 | 2.72 | 2.52 | 2.26 | [54] |
| 2152 | CN1CCCC1=O | C1CCCCC1 | 1.74 | 1.84 | 1.84 | 2.09 | 2.10 | 1.18 | 1.37 | 1.95 | 2.18 | [147 , 54 , 47] |
| 2153 | CN1CCCC1=O | CCCC(C)C | 1.99 | 2.22 | 2.19 | 2.33 | 2.63 | | | 2.86 | 2.54 | [54] |
| 2154 | CN1CCCC1=O | CCCCCCC | 2.32 | 2.50 | 2.48 | 2.54 | 2.97 | 1.95 | 2.25 | 2.88 | 2.94 | [147 , 54 , 164] |
| 2155 | CN1CCCC1=O | CC(C)CC(C)C | 2.18 | 2.49 | 2.48 | 2.54 | 2.85 | | | 3.23 | 2.78 | [54] |
| 2156 | CN1CCCC1=O | C1CCCCCC1 | 1.93 | 2.14 | 2.14 | 2.46 | 2.28 | | | 2.14 | 2.35 | [147] |
| 2157 | CN1CCCC1=O | CCCCCCCC | 2.58 | 2.75 | 2.77 | 2.76 | 3.32 | 2.15 | 2.15 | 3.08 | 3.15 | [147 , 54] |
| 2158 | CN1CCCC1=O | C1CCCCCCC1 | 2.10 | 2.41 | 2.44 | 2.83 | 2.52 | 1.53 | 1.01 | 2.35 | 2.38 | [147] |
| 2159 | CN1CCCC1=O | CC(C)C(C)C(C)C | 2.31 | 2.74 | 2.77 | 2.76 | 2.95 | | | | 2.81 | [54] |
| 2160 | CN1CCCC1=O | CC(C)CCC(C)C | 2.47 | 2.75 | 2.77 | 2.76 | | | | | 3.01 | [54] |
| 2161 | CN1CCCC1=O | CCC1CCCCC1 | 2.22 | 2.40 | 2.43 | 2.40 | | | | 2.58 | 2.56 | [54] |
| 2162 | CN1CCCC1=O | CCCCCCCCC | 2.84 | 3.00 | 3.05 | 2.96 | 3.75 | 2.34 | 2.04 | 3.27 | 3.28 | [54] |
| 2163 | CN1CCCC1=O | CCCCC=C | 1.35 | 1.55 | 1.52 | 1.66 | 2.24 | 1.55 | 2.58 | 2.12 | 2.07 | [147] |
| 2164 | CN1CCCC1=O | CCCCCC=C | 1.57 | 1.82 | 1.80 | 1.89 | 2.47 | 1.44 | 2.27 | | 2.25 | [147] |
| 2165 | CN1CCCC1=O | CCCCCCC=C | 1.90 | 2.07 | 2.09 | 2.11 | 2.83 | 1.54 | 2.13 | 2.42 | 2.39 | [147] |
| 2166 | CN1CCCC1=O | CCCCC#C | -0.06 | 0.64 | 0.63 | 0.79 | | | | | 0.35 | [147] |
| 2167 | CN1CCCC1=O | CCCCCC#C | 0.16 | 0.80 | 0.82 | 0.97 | | | | | 0.51 | [147] |
| 2168 | CN1CCCC1=O | CCCCCCC#C | 0.39 | 0.96 | 1.02 | 1.15 | | | | | 0.80 | [147] |
| 2169 | CN1CCCC1=O | CC=C(C)C | 1.05 | 1.59 | 1.50 | 1.56 | | 0.94 | 2.40 | | 1.68 | [47] |
| 2170 | CN1CCCC1=O | CC(=C)C=C | 0.56 | 0.77 | 0.76 | 0.52 | 1.24 | | | | 0.87 | [47] |
| 2171 | CCCCCCCCC | CCCCC | -0.04 | -0.12 | -0.05 | -0.02 | -0.02 | -0.29 | -0.22 | -0.04 | -0.05 | [54 , 61] |
| 2172 | CCCCCCCCC | CCCCCC | -0.02 | -0.06 | -0.03 | -0.01 | 0.05 | -0.26 | -0.24 | -0.04 | 0.01 | [54 , 61] |
| 2173 | CCCCCCCCC | C1CCCCC1 | -0.04 | -0.08 | -0.04 | 0.01 | -0.06 | -0.31 | -0.26 | -0.08 | -0.02 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2174 | CCCCCCCCC | CCCC(C)C | -0.02 | -0.06 | -0.03 | -0.01 | 0.09 | | | 0.01 | 0.01 | [54 , 61] |
| 2175 | CCCCCCCCC | CCCCCCC | -0.01 | -0.02 | -0.01 | -0.01 | 0.11 | -0.24 | -0.24 | -0.03 | 0.03 | [54 , 61] |
| 2176 | CCCCCCCCC | CC(C)CC(C)C | -0.01 | -0.02 | -0.01 | -0.01 | 0.17 | | | 0.07 | 0.04 | [54 , 61] |
| 2177 | CCCCCCCCC | CCCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.23 | -0.21 | -0.21 | -0.02 | 0.09 | [54 , 61] |
| 2178 | CCCCCCCCC | CC(C)C(C)C(C)C | 0.00 | -0.01 | 0.00 | 0.00 | -0.05 | | | | 0.03 | [54 , 61] |
| 2179 | CCCCCCCCC | CC(C)CCC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | | | | | 0.06 | [54] |
| 2180 | CCCCCCCCC | CCC1CCCCC1 | -0.01 | 0.01 | -0.01 | 0.03 | | | | -0.01 | 0.03 | [54 , 61] |
| 2181 | CCCCCCCCC | CCC(C)CCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | | | | | 0.06 | [61] |
| 2182 | CCCCCCCCCCCCCCCCC | CCc1ccccc1 | 0.29 | -0.09 | 0.04 | -0.05 | | -0.49 | -0.29 | 0.00 | 0.04 | [61] |
| 2183 | CCCCCCCCCCCCCCCCC | CCCc1ccccc1 | 0.29 | -0.05 | 0.05 | -0.01 | | | | | 0.07 | [61] |
| 2184 | CCCCCCCCCCCCCCCCC | C1CCOC1 | 0.23 | 0.02 | 0.22 | 0.02 | | -0.34 | 0.43 | -0.02 | 0.10 | [61] |
| 2185 | CCCCCCCCCCCCCCCCC | ClCCl | 0.34 | -0.30 | 0.10 | 0.32 | | -0.63 | 0.94 | 0.17 | 0.33 | [61] |
| 2186 | CCCCCCCCCCCCCCCCC | Clc1ccccc1 | 0.36 | 0.07 | 0.25 | -0.03 | | -0.37 | 0.66 | 0.00 | 0.16 | [61] |
| 2187 | CCCCCCCCCCCCCCCCC | Brc1ccccc1 | 1.09 | 1.12 | 1.28 | 0.88 | | 0.07 | 2.94 | 0.16 | 0.29 | [61] |
| 2188 | CCCCCCCC | CCCCC | -0.03 | -0.07 | -0.04 | -0.01 | 0.10 | -0.26 | -0.22 | -0.03 | -0.02 | [54 , 61 , 61] |
| 2189 | CCCCCCCC | CCCCCC | -0.01 | -0.03 | -0.01 | -0.01 | 0.20 | -0.25 | -0.24 | -0.03 | 0.02 | [54 , 61 , 178] |
| 2190 | CCCCCCCC | C1CCCCC1 | -0.02 | -0.04 | -0.03 | 0.03 | 0.02 | -0.27 | -0.21 | -0.02 | 0.04 | [54 , 61 , 128 , 128] |
| 2191 | CCCCCCCC | CCCC(C)C | -0.01 | -0.03 | -0.01 | -0.01 | 0.23 | | | 0.01 | 0.03 | [54 , 61] |
| 2192 | CCCCCCCC | CCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.29 | -0.22 | -0.22 | -0.02 | 0.05 | [54 , 61] |
| 2193 | CCCCCCCC | CC(C)CC(C)C | 0.00 | -0.01 | 0.00 | 0.00 | 0.32 | | | 0.06 | 0.07 | [54 , 61] |
| 2194 | CCCCCCCC | CC(C)C(C)C(C)C | 0.00 | 0.00 | 0.00 | 0.00 | 0.13 | | | | 0.06 | [54 , 61] |
| 2195 | CCCCCCCC | CC(C)CCC(C)C | 0.00 | 0.00 | 0.00 | 0.00 | | | | | 0.08 | [54] |
| 2196 | CCCCCCCC | CCC1CCCCC1 | 0.00 | 0.03 | 0.00 | 0.06 | | | | 0.03 | 0.01 | [54 , 61] |
| 2197 | CCCCCCCC | CCCCCCCCC | 0.00 | -0.01 | 0.00 | 0.00 | 0.63 | -0.17 | -0.16 | 0.01 | 0.09 | [54 , 61] |
| 2198 | CCCCCCCC | c1ccccc1 | 0.48 | 0.33 | 0.33 | 0.42 | 0.44 | -0.19 | 0.20 | 0.37 | 0.51 | [78 , 110] |
| 2199 | CCCCCCCC | CCCC=C | 0.01 | -0.02 | 0.04 | 0.00 | 0.15 | -0.14 | -0.25 | -0.07 | -0.04 | [61] |
| 2200 | CCCCCCCC | CC(C)C=C | 0.01 | -0.02 | 0.04 | 0.00 | | | | | -0.06 | [61] |
| 2201 | CCCCCCCC | CC(=C)C=C | 0.25 | 0.06 | 0.14 | 0.22 | 0.19 | | | | -0.01 | [61] |
| 2202 | CCCCCCCC | CCCC#CC | 0.28 | 0.15 | 0.17 | 0.30 | | | | | 0.51 | [82] |
| 2203 | CCCCCCCC | CCC#CCC | 0.23 | 0.15 | 0.17 | 0.30 | | | | | 0.72 | [82] |
| 2204 | CCCCCCCC | CO | 4.38 | 2.87 | 3.10 | 4.23 | 4.17 | 0.78 | 12.23 | 5.27 | 4.30 | [61] |
| 2205 | CCCCCCCC | CCO | 4.19 | 3.22 | 3.17 | 3.80 | 3.78 | 1.01 | 7.37 | 4.35 | 3.86 | [61] |
| 2206 | CCCCCCCC | CCCCO | 3.82 | 2.88 | 2.82 | 3.52 | 3.50 | 1.19 | 3.50 | 3.86 | 3.39 | [61] |
| 2207 | CCCCCCCC | CCC(C)O | 3.34 | 2.87 | 2.82 | 3.28 | 3.17 | 0.97 | 2.55 | 3.39 | 3.14 | [61] |
| 2208 | CCCCCCCC | CC(C)CO | 3.55 | 2.87 | 2.82 | 3.52 | 3.47 | 1.22 | 2.98 | 3.71 | 3.68 | [61] |
| 2209 | CCCCCCCC | CC(C)(C)O | 3.46 | 2.60 | 2.53 | 2.79 | | 1.03 | 2.20 | 3.12 | 2.88 | [61] |
| 2210 | CCCCCCCC | CCOC(=O)C | 1.25 | 1.06 | 1.10 | 1.21 | 1.47 | 0.09 | 0.23 | 1.62 | 1.16 | [61] |
| 2211 | CCCCCCCC | C1CCOC1 | 0.46 | 0.43 | 0.44 | 0.28 | 0.23 | 0.08 | 0.60 | 0.39 | 0.40 | [61] |
| 2212 | CCCCCCCC | CC(C)=O | 2.02 | 1.72 | 1.82 | 1.71 | 1.96 | 0.22 | 0.81 | 1.80 | 1.93 | [61 , 94] |
| 2213 | CCCCCCCC | CCC(C)=O | 1.65 | 1.59 | 1.65 | 1.59 | 1.58 | 0.20 | 0.44 | 1.37 | 1.40 | [61] |
| 2214 | CCCCCCCC | CCCCl | 0.47 | 0.06 | 0.14 | 0.25 | 0.44 | | | | 0.38 | [61] |
| 2215 | CCCCCCCC | ClCCl | 0.63 | 0.25 | 0.41 | 0.63 | 0.63 | -0.14 | 0.90 | 0.65 | 0.75 | [61] |
| 2216 | CCCCCCCC | ClC(Cl)Cl | 0.29 | 0.28 | 0.39 | 0.36 | 0.41 | -0.13 | | 0.38 | 0.35 | [61] |
| 2217 | CCCCCCCC | CCBr | 0.81 | 0.46 | 0.59 | 0.38 | 0.32 | -0.12 | | | 0.48 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2218 | CCCCCCCC | CCC#N | 2.87 | 2.10 | 2.22 | 2.26 | 2.72 | 0.48 | 1.98 | 2.59 | 2.99 | [61] |
| 2219 | CCCCCCCC | CCCC#N | 2.48 | 1.96 | 2.03 | 2.14 | | 0.55 | 1.18 | 2.13 | 2.72 | [98] |
| 2220 | CCCCCCCC | C[N+]([O-])=O | 3.44 | 3.56 | 3.73 | 2.92 | 3.40 | 0.59 | 5.38 | 3.37 | 3.61 | [61] |
| 2221 | CCCCCCCC | CC[N+]([O-])=O | 2.79 | 2.54 | 2.64 | 1.96 | | 0.63 | 2.93 | | 2.90 | [61] |
| 2222 | CCCCCCCC | CCI | 0.85 | 0.54 | 0.65 | 0.60 | 0.57 | | | | 0.58 | [61] |
| 2223 | CCCCCCCC | C(=S)=S | 0.37 | 0.15 | 0.34 | 0.23 | | -0.21 | 1.07 | | 0.23 | [61] |
| 2224 | CCCCCCCCO | CCCCC | 0.68 | 0.50 | 0.57 | 0.84 | 1.06 | 0.94 | 2.05 | 0.95 | 0.83 | [166 , 54 , 61 , 61] |
| 2225 | CCCCCCCCO | CCCCCC | 0.81 | 0.67 | 0.70 | 0.93 | 1.18 | 1.11 | 1.79 | 1.09 | 0.97 | [166 , 54 , 61 , 61 , 68] |
| 2226 | CCCCCCCCO | CCCCCCC | 0.92 | 0.82 | 0.82 | 1.02 | 1.29 | 1.28 | 1.55 | 1.25 | 1.09 | [166 , 54 , 61 , 61 , 68 , 67] |
| 2227 | CCCCCCCCO | CCCCCCCC | 1.03 | 0.95 | 0.93 | 1.11 | 1.45 | 1.46 | 1.44 | 1.42 | 1.18 | [166 , 54 , 61 , 61 , 61] |
| 2228 | CCCCCCCCO | C1CCCCC1 | 0.67 | 0.58 | 0.57 | 0.83 | 1.01 | 0.77 | 0.59 | 0.96 | 0.79 | [54 , 61 , 61 , 68] |
| 2229 | CCCCCCCCO | CCCC(C)C | 0.78 | 0.67 | 0.70 | 0.93 | 1.21 | | | 1.13 | 0.96 | [54 , 61 , 61] |
| 2230 | CCCCCCCCO | CC(C)CC(C)C | 0.86 | 0.82 | 0.82 | 1.02 | 1.31 | | | 1.31 | 1.08 | [54 , 61 , 61] |
| 2231 | CCCCCCCCO | CC(C)C(C)C(C)C | 0.91 | 0.95 | 0.92 | 1.11 | 1.16 | | | | 1.08 | [54 , 61 , 61] |
| 2232 | CCCCCCCCO | CC(C)CCC(C)C | 0.98 | 0.95 | 0.93 | 1.11 | | | | | 1.22 | [54] |
| 2233 | CCCCCCCCO | CCC1CCCCC1 | 0.89 | 0.90 | 0.81 | 0.96 | | | | 1.32 | 0.98 | [54 , 61 , 61] |
| 2234 | CCCCCCCCO | CCCCCCCCC | 1.14 | 1.06 | 1.03 | 1.18 | 1.69 | 1.64 | 1.34 | 1.57 | 1.32 | [54 , 61 , 61] |
| 2235 | CCCCCCCCO | CCC(C)CCC(C)C | 1.07 | 1.06 | 1.03 | 1.18 | | | | | 1.11 | [61] |
| 2236 | CCCCCCCCO | c1ccccc1 | 0.55 | 0.47 | 0.43 | 0.67 | 0.77 | 0.41 | -0.12 | 0.55 | 0.73 | [61] |
| 2237 | CCCCCCCCO | Cc1ccccc1 | 0.68 | 0.62 | 0.49 | 0.67 | 0.81 | 0.51 | 0.05 | 0.67 | 0.69 | [61] |
| 2238 | CCCCCCCCO | Cc1cccc(C)c1 | 0.74 | 0.69 | 0.51 | 0.67 | 0.90 | 0.53 | 0.12 | | 0.85 | [61] |
| 2239 | CCCCCCCCO | Cc1ccccc1C | 0.72 | 0.69 | 0.51 | 0.67 | 0.89 | 0.51 | 0.11 | | 0.87 | [61] |
| 2240 | CCCCCCCCO | CCc1ccccc1 | 0.77 | 0.74 | 0.58 | 0.84 | 0.93 | 0.79 | 0.20 | 0.93 | 0.91 | [61] |
| 2241 | CCCCCCCCO | CCCc1ccccc1 | 0.85 | 0.85 | 0.67 | 0.94 | 1.00 | | | | 1.02 | [61] |
| 2242 | CCCCCCCCO | CC(=C)C=C | 0.52 | 0.45 | 0.57 | 0.45 | 0.81 | | | | 0.63 | [61] |
| 2243 | CCCCCCCCO | CCCCC=C | 0.63 | 0.65 | 0.68 | 0.79 | 1.01 | 0.99 | 1.89 | 0.98 | 0.93 | [61] |
| 2244 | CCCCCCCCO | CCCCCCC=C | 0.85 | 0.92 | 0.90 | 0.98 | 1.22 | 0.79 | 1.41 | 1.18 | 1.10 | [61] |
| 2245 | CCCCCCCCO | CCCCCCCC=C | 0.96 | 1.04 | 1.00 | 1.06 | | | | | 1.18 | [61] |
| 2246 | CCCCCCCCC#N | CCCCC | 0.69 | 0.44 | 0.49 | 0.83 | | 0.11 | 0.15 | | 0.64 | [61] |
| 2247 | CCCCCCCCC#N | CCCCCC | 0.82 | 0.58 | 0.61 | 0.90 | | 0.20 | 0.06 | | 0.79 | [61 , 98 , 47] |
| 2248 | CCCCCCCCC#N | C1CCCCC1 | 0.65 | 0.45 | 0.49 | 0.72 | | 0.10 | -0.33 | | 0.64 | [61 , 98 , 47] |
| 2249 | CCCCCCCCC#N | CCCC(C)C | 0.78 | 0.58 | 0.60 | 0.90 | | | | | 0.76 | [61] |
| 2250 | CCCCCCCCC#N | CCCCCCC | 0.94 | 0.70 | 0.71 | 0.98 | | 0.29 | -0.01 | | 0.83 | [61] |
| 2251 | CCCCCCCCC#N | CC(C)CC(C)C | 0.87 | 0.70 | 0.71 | 0.98 | | | | | 0.87 | [61] |
| 2252 | CCCCCCCCC#N | CCCCCCCC | 1.05 | 0.81 | 0.81 | 1.04 | | 0.37 | -0.03 | | 0.99 | [61 , 61] |
| 2253 | CCCCCCCCC#N | CC(C)C(C)C(C)C | 0.92 | 0.81 | 0.81 | 1.04 | | | | | 0.81 | [61] |
| 2254 | CCCCCCCCC#N | CCC1CCCCC1 | 0.87 | 0.71 | 0.70 | 0.84 | | | | | 0.79 | [61] |
| 2255 | CCCCCCCCC#N | CCCCCCCCC | 1.16 | 0.90 | 0.90 | 1.11 | | 0.45 | -0.05 | | 1.13 | [61] |
| 2256 | CCCCCCCCC#N | CCC(C)CCC(C)C | 1.09 | 0.90 | 0.90 | 1.11 | | | | | 0.93 | [61] |
| 2257 | CCCCCCCCC#N | c1ccccc1 | -0.04 | -0.17 | -0.14 | -0.11 | | 0.05 | -0.27 | | -0.22 | [61 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2258 | CCCCCCCCC#N | Cc1ccccc1 | 0.09 | 0.03 | 0.02 | -0.05 | | 0.04 | -0.26 | | -0.17 | [61] |
| 2259 | CCCCCCCCC#N | CC=C(C)C | 0.29 | 0.28 | 0.31 | 0.52 | | -0.17 | -0.03 | | 0.45 | [47] |
| 2260 | CCCCCCCCC#N | CC(=C)C=C | 0.12 | -0.02 | 0.10 | 0.10 | | | | | 0.15 | [61 , 47] |
| 2261 | CCCCCCCCC#N | CCO | 1.59 | 0.92 | 0.88 | 1.76 | | 0.26 | 5.46 | | 1.31 | [61] |
| 2262 | CCCCCCCCC#N | C1COCCO1 | -0.05 | 0.24 | 0.02 | 0.18 | | 0.04 | 0.35 | | -0.02 | [61] |
| 2263 | CCCCCCCCC#N | CCC(C)=O | 0.00 | -0.20 | -0.13 | -0.01 | | -0.36 | -0.14 | | -0.08 | [61] |
| 2264 | CCCCCCCCCCCCCCC | c1ccccc1 | 0.29 | -0.05 | 0.15 | 0.10 | | | | | 0.08 | [185] |
| 2265 | CCCCC=O | C1CCCCC1 | 0.86 | 1.24 | 1.24 | 0.95 | | 0.63 | 0.06 | | 0.88 | [71] |
| 2266 | CCCCC | CCCCCC | 0.00 | -0.01 | -0.01 | 0.00 | 0.25 | -0.16 | -0.15 | 0.02 | 0.08 | [54 , 61] |
| 2267 | CCCCC | C1CCCCC1 | 0.01 | 0.05 | 0.00 | 0.14 | 0.24 | -0.07 | 0.04 | 0.22 | 0.23 | [54 , 61] |
| 2268 | CCCCC | CCCC(C)C | 0.00 | -0.01 | -0.01 | 0.00 | 0.29 | | | 0.01 | -0.02 | [54] |
| 2269 | CCCCC | CCCCCCC | -0.02 | -0.05 | -0.02 | 0.00 | 0.33 | -0.12 | -0.11 | 0.04 | 0.11 | [54 , 61] |
| 2270 | CCCCC | CC(C)CC(C)C | -0.02 | -0.04 | -0.02 | 0.00 | 0.37 | | | 0.00 | 0.09 | [54 , 61] |
| 2271 | CCCCC | CCCCCCCC | -0.04 | -0.09 | -0.04 | 0.00 | 0.46 | -0.08 | -0.07 | 0.04 | 0.17 | [54 , 61 , 61] |
| 2272 | CCCCC | CC(C)C(C)C(C)C | -0.03 | -0.09 | -0.04 | 0.00 | 0.17 | | | | 0.16 | [54 , 61] |
| 2273 | CCCCC | CC(C)CCC(C)C | -0.04 | -0.09 | -0.04 | 0.00 | | | | | 0.15 | [54] |
| 2274 | CCCCC | CCC1CCCCC1 | 0.00 | 0.00 | -0.03 | 0.15 | | | | 0.22 | 0.31 | [54 , 61] |
| 2275 | CCCCC | CCCCCCCCC | -0.06 | -0.16 | -0.07 | -0.01 | 0.67 | -0.04 | -0.04 | 0.04 | 0.27 | [54 , 61] |
| 2276 | CCCCC | CCC(C)CCC(C)C | -0.06 | -0.15 | -0.07 | -0.01 | | | | | 0.08 | [61] |
| 2277 | CCCCC | c1ccccc1 | 0.60 | 0.51 | 0.39 | 0.65 | 0.83 | 0.09 | 0.48 | 0.63 | 0.68 | [78] |
| 2278 | CCCCC | Cc1ccccc1 | 0.59 | 0.52 | 0.37 | 0.65 | 0.83 | 0.14 | 0.41 | 0.60 | 0.62 | [61 , 186] |
| 2279 | CCCCC | C1COCCO1 | 1.21 | 1.96 | 1.74 | 1.27 | 1.36 | 0.44 | 1.38 | 1.62 | 1.56 | [61] |
| 2280 | CCCCC | CCC(C)=O | 1.76 | 1.71 | 1.71 | 1.80 | 1.73 | 0.36 | 0.70 | 1.48 | 1.70 | [61] |
| 2281 | CCCCC | O=C1CCCCC1 | 1.63 | 0.99 | 0.95 | 1.38 | 1.64 | 0.46 | 0.97 | 0.70 | 0.67 | [135] |
| 2282 | CCCCC | CCCC#N | 2.62 | 2.09 | 2.09 | 2.46 | | 0.70 | 1.35 | 2.26 | 2.09 | [98] |
| 2283 | CCCCCO | CCCCC | 1.12 | 0.94 | 0.92 | 1.24 | 1.31 | 1.47 | 2.23 | 1.40 | 1.44 | [166 , 61] |
| 2284 | CCCCCO | CCCCCC | 1.29 | 1.13 | 1.09 | 1.35 | 1.45 | 1.68 | 2.01 | 1.55 | 1.43 | [166 , 61 , 91] |
| 2285 | CCCCCO | CCCCCCC | 1.44 | 1.29 | 1.23 | 1.46 | 1.60 | 1.91 | 1.79 | 1.71 | 1.54 | [166] |
| 2286 | CCCCCO | CCCC(C)C | 1.24 | 1.13 | 1.08 | 1.35 | 1.47 | | | 1.60 | 1.25 | [91] |
| 2287 | CCCCCO | CCC(C)CC | 1.23 | 1.13 | 1.08 | 1.35 | 1.42 | | | | 1.30 | [91] |
| 2288 | CCCCCO | CC(C)C(C)C | 1.18 | 1.13 | 1.08 | 1.35 | 1.38 | | | 1.59 | 1.40 | [91] |
| 2289 | CCCCCO | CCC(C)(C)C | 1.17 | 1.13 | 1.11 | 1.35 | 1.38 | | | | 1.45 | [91] |
| 2290 | CCCCCO | CCCCCCCC | 1.59 | 1.44 | 1.37 | 1.56 | 1.78 | 2.14 | 1.69 | 1.87 | 1.80 | [61] |
| 2291 | CCCCCO | c1ccccc1 | 0.81 | 0.86 | 0.65 | 1.02 | 1.03 | 0.84 | 0.26 | 0.87 | 1.12 | [61] |
| 2292 | CCCCCO | Cc1ccccc1 | 0.99 | 1.00 | 0.72 | 1.03 | 1.09 | 0.96 | 0.42 | 1.00 | 1.10 | [61] |
| 2293 | CCCO | CCCCC | 1.66 | 1.42 | 1.34 | 1.72 | 1.93 | 2.39 | 2.79 | 1.85 | 1.67 | [166 , 54 , 61 , 61] |
| 2294 | CCCO | CCCCCC | 1.88 | 1.64 | 1.54 | 1.87 | 2.13 | 2.71 | 2.58 | 2.03 | 1.96 | [166 , 54 , 61 , 61 , 63] |
| 2295 | CCCO | CCCCCCC | 2.09 | 1.83 | 1.73 | 2.02 | 2.32 | 3.04 | 2.37 | 2.21 | 2.05 | [166 , 54 , 61 , 63] |
| 2296 | CCCO | CCCCCCCC | 2.29 | 2.01 | 1.91 | 2.16 | 2.56 | 3.38 | 2.27 | 2.39 | 2.23 | [166 , 54 , 61 , 61 , 61] |
| 2297 | CCCO | C1CCCCC1 | 1.65 | 1.58 | 1.30 | 1.78 | 1.98 | 2.14 | 1.58 | 1.89 | 1.75 | [54] |
| 2298 | CCCO | CCCC(C)C | 1.81 | 1.64 | 1.53 | 1.87 | 2.13 | | | 2.06 | 1.85 | [54 , 61 , 61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2299 | CCCO | CC(C)CC(C)C | 1.94 | 1.83 | 1.72 | 2.02 | 2.28 | | | 2.26 | 1.99 | [54 , 61 , 61] |
| 2300 | CCCO | CC(C)C(C)C(C)C | 2.04 | 2.01 | 1.91 | 2.16 | 2.23 | | | | 2.07 | [54 , 61 , 61] |
| 2301 | CCCO | CC(C)CCC(C)C | 2.17 | 2.01 | 1.91 | 2.16 | | | | | 2.15 | [54] |
| 2302 | CCCO | CCC1CCCCC1 | 2.17 | 1.99 | 1.68 | 1.99 | | | | 2.29 | 2.05 | [54 , 61 , 61] |
| 2303 | CCCO | CCCCCCCCC | 2.49 | 2.17 | 2.09 | 2.30 | 2.88 | 3.72 | 2.18 | 2.56 | 2.44 | [54 , 61 , 61 , 86] |
| 2304 | CCCO | CCC(C)CCC(C)C | 2.34 | 2.18 | 2.09 | 2.30 | | | | | 2.11 | [61] |
| 2305 | CCCO | c1ccccc1 | 1.14 | 1.28 | 0.89 | 1.42 | 1.47 | 1.50 | 0.86 | 1.34 | 1.73 | [89] |
| 2306 | CCCO | Cc1ccccc1 | 1.37 | 1.43 | 0.97 | 1.46 | 1.59 | 1.70 | 1.02 | 1.47 | 1.32 | [61 , 89] |
| 2307 | CCCO | Cc1cccc(C)c1 | 1.51 | 1.51 | 1.01 | 1.51 | 1.76 | 1.78 | 1.06 | | 2.06 | [89] |
| 2308 | CCCO | Cc1ccc(C)cc1 | 1.52 | 1.51 | 1.01 | 1.51 | 1.69 | 1.75 | 1.14 | 1.62 | 1.62 | [89] |
| 2309 | CCCO | Cc1cccc1C | 1.46 | 1.51 | 1.01 | 1.51 | 1.75 | 1.73 | 1.06 | | 2.79 | [89] |
| 2310 | CCCCCCCCCCCCCCCCCCCCCCCC | CCCCCCC | -0.19 | -0.46 | -0.24 | -0.20 | | | | | -0.21 | [61] |
| 2311 | CCCCCCCCCCCCC | C1CCCCC1 | -0.14 | -0.30 | -0.15 | -0.11 | | -0.51 | -0.48 | -0.30 | -0.17 | [128] |
| 2312 | CCCCCCCCCCCCC | c1ccccc1 | 0.31 | 0.00 | 0.17 | 0.14 | | -0.49 | -0.06 | 0.08 | 0.16 | [111 , 187] |
| 2313 | CCCCCCCC#N | CCCCCC | 0.96 | 0.70 | 0.72 | 1.02 | | 0.36 | 0.21 | | 1.00 | [98 , 47] |
| 2314 | CCCCCCCC#N | C1CCCCC1 | 0.78 | 0.57 | 0.59 | 0.83 | | 0.24 | -0.26 | | 0.84 | [98 , 47] |
| 2315 | CCCCCCCC#N | c1ccccc1 | 0.00 | -0.11 | -0.09 | -0.04 | | 0.17 | -0.31 | | -0.12 | [47] |
| 2316 | CCCCCCCC#N | CC=C(C)C | 0.39 | 0.39 | 0.41 | 0.63 | | -0.07 | 0.12 | | 0.52 | [47] |
| 2317 | CCCCCCCC#N | CC(=C)C=C | 0.19 | 0.08 | 0.16 | 0.15 | | | | | 0.17 | [47] |
| 2318 | CCCCCCCCN | CCCCCCC | 0.47 | 0.35 | 0.36 | 0.54 | | 0.29 | 0.06 | | 0.52 | [137] |
| 2319 | N#CCCOCCC#N | CCCCCC | 4.63 | 2.94 | 2.94 | 4.06 | | | | | 5.44 | [47 , 73] |
| 2320 | N#CCCOCCC#N | c1ccccc1 | 1.69 | 0.68 | 0.63 | 1.16 | | | | | 1.72 | [47 , 73] |
| 2321 | CCCCCCCCCCCCCCCC#N | CCCCC | 0.23 | -0.08 | 0.10 | 0.38 | | | | | 0.23 | [54 , 61] |
| 2322 | CCCCCCCCCCCCCCCC#N | CCCCCC | 0.32 | 0.06 | 0.19 | 0.44 | | | | | 0.36 | [54 , 61] |
| 2323 | CCCCCCCCCCCCCCCC#N | C1CCCCC1 | 0.19 | -0.07 | 0.10 | 0.27 | | | | | 0.18 | [54 , 61] |
| 2324 | CCCCCCCCCCCCCCCC#N | CCCC(C)C | 0.30 | 0.06 | 0.19 | 0.44 | | | | | 0.37 | [54 , 61] |
| 2325 | CCCCCCCCCCCCCCCC#N | CCCCCCC | 0.40 | 0.17 | 0.27 | 0.51 | | | | | 0.39 | [54 , 61] |
| 2326 | CCCCCCCCCCCCCCCC#N | CC(C)CC(C)C | 0.36 | 0.17 | 0.27 | 0.51 | | | | | 0.49 | [54 , 61] |
| 2327 | CCCCCCCCCCCCCCCC#N | CCCCCCCC | 0.47 | 0.28 | 0.35 | 0.56 | | | | | 0.54 | [54 , 61 , 61] |
| 2328 | CCCCCCCCCCCCCCCC#N | CC(C)C(C)C(C)C | 0.39 | 0.28 | 0.34 | 0.56 | | | | | 0.38 | [54 , 61] |
| 2329 | CCCCCCCCCCCCCCCC#N | CC(C)CCC(C)C | 0.44 | 0.28 | 0.34 | 0.56 | | | | | 0.62 | [54] |
| 2330 | CCCCCCCCCCCCCCCC#N | CCC1CCCCC1 | 0.34 | 0.19 | 0.28 | 0.37 | | | | | 0.33 | [54 , 61] |
| 2331 | CCCCCCCCCCCCCCCC#N | CCCCCCCCC | 0.54 | 0.36 | 0.41 | 0.62 | | | | | 0.66 | [54 , 61] |
| 2332 | CCCCCCCCCCCCCCCC#N | CCC(C)CCC(C)C | 0.50 | 0.36 | 0.41 | 0.62 | | | | | 0.55 | [61] |
| 2333 | CCCCCCCCCCCCCCCC#N | Cc1ccccc1 | -0.08 | -0.27 | -0.14 | -0.31 | | | | | -0.36 | [61] |
| 2334 | CCCCCCCCCCCCCCCC#N | CCO | 1.73 | 1.01 | 1.10 | 1.85 | | | | | 1.48 | [61] |
| 2335 | CCCCCCCCCCCCCCCC#N | C1COCCO1 | -0.01 | 0.25 | 0.11 | 0.10 | | | | | 0.02 | [61] |
| 2336 | CCCCCCCCCCCCCCCC#N | CCC(C)=O | 0.17 | -0.19 | 0.02 | 0.03 | | | | | -0.02 | [61] |
| 2337 | CCCCC#N | CCCCCC | 1.68 | 1.24 | 1.24 | 1.55 | | 1.00 | 0.73 | | 1.55 | [98 , 47] |
| 2338 | CCCCC#N | C1CCCCC1 | 1.42 | 1.09 | 1.05 | 1.35 | | 0.80 | 0.11 | | 1.46 | [98 , 47] |
| 2339 | CCCCC#N | c1ccccc1 | 0.27 | 0.19 | 0.10 | 0.22 | | 0.66 | -0.20 | | 0.07 | [101 , 47] |
| 2340 | CCCCC#N | CC=C(C)C | 0.89 | 0.85 | 0.83 | 1.05 | | 0.36 | 0.66 | | 1.04 | [47] |
| 2341 | CCCCC#N | CC(=C)C=C | 0.54 | 0.43 | 0.44 | 0.40 | | | | | 0.62 | [47] |
| 2342 | CCCCCN | CCCCCCC | 0.82 | 0.63 | 0.64 | 0.77 | | 0.55 | 0.10 | | 0.79 | [137] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2343 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCC | 2.67 | 2.16 | 2.09 | 2.31 | | -0.05 | 0.39 | | 2.10 | [63] |
| 2344 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCC | 1.95 | 1.52 | 1.54 | 1.92 | | | | | 1.53 | [54] |
| 2345 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCC | 2.34 | 1.87 | 1.83 | 2.11 | | | | | 1.94 | [54 , 63 , 188 , 188] |
| 2346 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | C1CCCCC1 | 2.13 | 1.67 | 1.52 | 1.55 | | | | | 2.29 | [54] |
| 2347 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCC(C)C | 2.26 | 1.87 | 1.83 | 2.11 | | | | | 1.84 | [54] |
| 2348 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCC | 2.71 | 2.21 | 2.11 | 2.29 | | | | | 2.44 | [54 , 188] |
| 2349 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)CC(C)C | 2.53 | 2.21 | 2.11 | 2.29 | | | | | 2.06 | [54] |
| 2350 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCCC | 3.09 | 2.53 | 2.39 | 2.47 | | | | | 2.90 | [54] |
| 2351 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)C(C)C(C)C | 2.76 | 2.53 | 2.38 | 2.47 | | | | | 2.43 | [54] |
| 2352 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)CCC(C)C | 2.90 | 2.53 | 2.38 | 2.47 | | | | | 2.49 | [54] |
| 2353 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCC1CCCCC1 | 2.80 | 2.36 | 2.08 | 1.85 | | | | | 2.95 | [54] |
| 2354 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCCCC | 3.46 | 2.83 | 2.65 | 2.65 | | | | | 3.31 | [54] |
| 2355 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCC | 1.86 | 1.38 | 1.47 | 1.89 | | | | | 1.49 | [54] |
| 2356 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCC | 2.26 | 1.75 | 1.78 | 2.10 | | | | | 1.94 | [54] |
| 2357 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | C1CCCCC1 | 2.04 | 1.53 | 1.45 | 1.54 | | | | | 2.20 | [54] |
| 2358 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCC(C)C | 2.17 | 1.75 | 1.78 | 2.10 | | | | | 1.79 | [54] |
| 2359 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCC | 2.63 | 2.11 | 2.07 | 2.31 | | | | | 2.43 | [54] |
| 2360 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)CC(C)C | 2.45 | 2.11 | 2.07 | 2.31 | | | | | 2.01 | [54] |
| 2361 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCCC | 3.01 | 2.44 | 2.36 | 2.51 | | | | | 2.83 | [54] |
| 2362 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)C(C)C(C)C | 2.68 | 2.44 | 2.35 | 2.51 | | | | | 2.36 | [54] |
| 2363 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CC(C)CCC(C)C | 2.82 | 2.44 | 2.35 | 2.51 | | | | | 2.45 | [54] |
| 2364 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCC1CCCCC1 | 2.72 | 2.25 | 2.04 | 1.88 | | | | | 2.83 | [54] |
| 2365 | FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F | CCCCCCCCC | 3.38 | 2.77 | 2.63 | 2.71 | | | | | 3.24 | [54] |
| 2366 | CC(C1=CC=CC=C1)O | CCCCCC | 1.78 | 1.21 | 1.21 | 1.74 | | | | | 2.28 | [47] |
| 2367 | CC(C1=CC=CC=C1)O | C1CCCCC1 | 1.47 | 0.96 | 1.00 | 1.57 | | | | | 1.76 | [47] |
| 2368 | CC(C1=CC=CC=C1)O | c1ccccc1 | 0.47 | 0.29 | 0.34 | 0.49 | | | | | 0.71 | [47] |
| 2369 | Oc1ccccc1 | CCCCCC | 2.35 | 2.05 | 1.92 | 2.74 | | 2.22 | 2.92 | 2.88 | 2.77 | [73 , 61 , 47] |
| 2370 | Oc1ccccc1 | c1ccccc1 | 0.67 | 0.59 | 0.59 | 0.80 | | 0.89 | 0.93 | 0.85 | 0.98 | [73 , 61 , 47] |
| 2371 | Oc1ccccc1 | CCCCC | 2.07 | 1.81 | 1.66 | 2.49 | | 1.99 | 3.17 | 2.66 | 2.54 | [61] |
| 2372 | Oc1ccccc1 | C1CCCCC1 | 1.94 | 1.64 | 1.62 | 1.84 | | 1.53 | 1.76 | 2.28 | 2.17 | [61 , 47] |
| 2373 | Oc1ccccc1 | CCCCCCC | 2.61 | 2.27 | 2.17 | 3.00 | | 2.44 | 2.68 | 3.12 | 2.93 | [61] |
| 2374 | Oc1ccccc1 | CC=C(C)C | 1.42 | 1.63 | 1.41 | 1.96 | | 1.08 | 2.85 | | 1.92 | [47] |
| 2375 | Oc1ccccc1 | CC(=C)C=C | 1.00 | 1.03 | 0.92 | 1.05 | | | | | 1.53 | [61 , 47] |
| 2376 | CC(=O)Cc1ccccc1 | CCCCC | 1.48 | 0.93 | 0.85 | 1.69 | | | | | 2.04 | [103 , 47] |
| 2377 | CC(=O)Cc1ccccc1 | CCC(C)C | 1.42 | 0.92 | 0.85 | 1.69 | | | | | 2.07 | [47] |
| 2378 | CC(=O)Cc1ccccc1 | CCCCCC | 1.72 | 1.10 | 1.01 | 1.85 | | | | | 2.15 | [103 , 47] |
| 2379 | CC(=O)Cc1ccccc1 | C1CCCCC1 | 1.40 | 0.83 | 0.84 | 1.72 | | | | | 1.66 | [47] |
| 2380 | CC(=O)Cc1ccccc1 | c1ccccc1 | 0.11 | -0.03 | 0.03 | 0.08 | | | | | 0.25 | [47] |
| 2381 | CC(=O)Cc1ccccc1 | CC=C(C)C | 0.87 | 0.77 | 0.63 | 1.25 | | | | | 1.41 | [47] |
| 2382 | CC(=O)Cc1ccccc1 | CC(=C)C=C | 0.41 | 0.31 | 0.30 | 0.50 | | | | | 0.90 | [47] |
| 2383 | C1CCNCC1 | C1CCCCC1 | 0.60 | 0.34 | 0.34 | 0.51 | | 0.47 | 0.30 | | 0.66 | [160] |
| 2384 | C1CCNCC1 | CCCCCCC | 0.78 | 0.47 | 0.44 | 0.75 | | 0.96 | 0.85 | | 0.90 | [137] |
| 2385 | CCC#N | CCCCCC | 2.81 | 1.87 | 1.97 | 2.22 | | 1.78 | 1.38 | 2.52 | 2.35 | [73 , 54 , 61 , 61 , 98 , 47] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2386 | CCC#N | c1ccccc1 | 0.84 | 0.52 | 0.36 | 0.57 | | 1.23 | 0.22 | 0.67 | 0.50 | [73 , 61 , 47] |
| 2387 | CCC#N | CCCCC | 2.47 | 1.68 | 1.72 | 2.09 | | 1.56 | 1.53 | 2.30 | 2.08 | [54 , 61 , 61 , 98 , 74] |
| 2388 | CCC#N | C1CCCCC1 | 2.42 | 1.69 | 1.67 | 2.04 | | 1.47 | 0.68 | 2.31 | 2.01 | [54 , 61 , 61 , 98] |
| 2389 | CCC#N | CCCC(C)C | 2.72 | 1.87 | 1.97 | 2.22 | | | | 2.55 | 2.34 | [54 , 61] |
| 2390 | CCC#N | CCCCCCC | 3.14 | 2.04 | 2.21 | 2.36 | | 2.02 | 1.23 | 2.75 | 2.59 | [54 , 61 , 61 , 98 , 98] |
| 2391 | CCC#N | CC(C)CC(C)C | 2.95 | 2.04 | 2.20 | 2.36 | | | | 2.81 | 2.52 | [54 , 61] |
| 2392 | CCC#N | CCCCCCCC | 3.47 | 2.19 | 2.44 | 2.50 | | 2.25 | 1.17 | 2.98 | 2.82 | [54 , 61 , 98] |
| 2393 | CCC#N | CC(C)C(C)C(C)C | 3.10 | 2.19 | 2.43 | 2.50 | | | | | 2.67 | [54 , 61] |
| 2394 | CCC#N | CC(C)CCC(C)C | 3.31 | 2.19 | 2.44 | 2.50 | | | | | 2.72 | [54] |
| 2395 | CCC#N | CCC1CCCCC1 | 3.01 | 2.05 | 2.15 | 2.25 | | | | 2.82 | 2.64 | [54 , 61] |
| 2396 | CCC#N | CCCCCCCCC | 3.79 | 2.34 | 2.67 | 2.64 | | 2.49 | 1.10 | 3.21 | 3.11 | [54 , 61] |
| 2397 | CCC#N | CCCC=C | 1.70 | 1.16 | 1.19 | 1.44 | | 1.06 | 1.53 | 1.71 | 1.50 | [61 , 74] |
| 2398 | CCC#N | CC(C)C=C | 1.68 | 1.16 | 1.19 | 1.44 | | | | | 1.48 | [61] |
| 2399 | CCC#N | CC(=C)C=C | 1.21 | 0.83 | 0.84 | 0.69 | | | | | 0.93 | [61] |
| 2400 | CCC#N | CCCCCC=C | 2.34 | 1.52 | 1.66 | 1.75 | | 1.49 | 1.24 | | 2.01 | [61] |
| 2401 | CCC#N | CCOC(=O)C | 0.18 | -0.02 | 0.01 | 0.25 | | 0.10 | 0.17 | 0.18 | 0.82 | [61 , 61] |
| 2402 | CCC#N | CCOCC | 1.01 | 0.62 | 0.64 | 0.87 | | 0.72 | 1.06 | 1.03 | 2.17 | [61] |
| 2403 | CCC#N | CC(C)=O | -0.06 | -0.22 | -0.24 | 0.01 | | -0.11 | -0.05 | 0.05 | 0.39 | [61] |
| 2404 | CCC#N | CCCCl | 0.52 | 0.45 | 0.46 | 0.82 | | | | | 0.62 | [61] |
| 2405 | CCC#N | CC(C)(C)Cl | 0.64 | 1.05 | 1.10 | 1.34 | | | | | 0.85 | [61] |
| 2406 | CCC#N | ClCCl | -0.73 | -0.09 | -0.09 | -0.24 | | 0.17 | -0.12 | -0.13 | -0.20 | [61] |
| 2407 | CCC#N | ClC(Cl)Cl | -0.65 | -0.16 | -0.19 | -0.11 | | 0.57 | | -0.15 | -0.12 | [61] |
| 2408 | CCC#N | ClC(Cl)(Cl)Cl | 0.68 | 0.82 | 0.84 | 1.12 | | 1.37 | 0.39 | 1.29 | 1.12 | [61] |
| 2409 | CCC#N | CCBr | -0.04 | 0.34 | 0.34 | 0.59 | | 0.05 | | | 0.54 | [61] |
| 2410 | CCC#N | CCI | 0.00 | 0.15 | 0.13 | 0.18 | | | | | 0.97 | [61] |
| 2411 | CCC#N | CCN(CC)CC | 2.03 | 1.08 | 1.23 | 1.70 | | 1.93 | 0.44 | 1.87 | 1.46 | [61] |
| 2412 | CCC#N | C(=S)=S | 0.67 | 1.51 | 1.47 | 1.56 | | 1.00 | -0.16 | | 1.68 | [61] |
| 2413 | CCC(=O)c1ccccc1 | CCCCCC | 1.20 | 1.01 | 0.92 | 1.52 | | | | | 1.52 | [61 , 116] |
| 2414 | CCC(=O)c1ccccc1 | C1CCCCC1 | 0.94 | 0.75 | 0.76 | 1.39 | | | | | 1.23 | [61 , 116] |
| 2415 | CCC(=O)c1ccccc1 | c1ccccc1 | 0.02 | -0.07 | -0.01 | -0.01 | | | | | 0.07 | [61 , 116] |
| 2416 | CCC(=O)c1ccccc1 | C1C=CC=C1 | 0.06 | 0.18 | 0.26 | 0.33 | | | | | 0.82 | [61 , 116] |
| 2417 | CCC(=O)c1ccccc1 | CC(=C)C=C | 0.25 | 0.36 | 0.34 | 0.39 | | | | | 0.53 | [61 , 116] |
| 2418 | CCC(=O)c1ccccc1 | CCOC(=O)C | 0.02 | -0.08 | -0.20 | 0.17 | | | | | 0.26 | [61 , 116] |
| 2419 | CCC(=O)c1ccccc1 | CC(C)=O | 0.17 | 0.04 | 0.01 | 0.01 | | | | | 0.27 | [61 , 116] |
| 2420 | CCC(=O)c1ccccc1 | CCCCl | 0.07 | -0.12 | -0.14 | 0.20 | | | | | 0.36 | [61 , 116] |
| 2421 | CCC(=O)c1ccccc1 | CC(C)(C)Cl | 0.15 | 0.39 | 0.29 | 0.70 | | | | | 0.71 | [61 , 116] |
| 2422 | CCC(=O)c1ccccc1 | ClCCCl | -0.20 | -0.36 | -0.36 | -0.27 | | | | | -0.19 | [116] |
| 2423 | CCC(=O)c1ccccc1 | ClC(Cl)Cl | -0.73 | -0.78 | -0.73 | -1.51 | | | | | -0.62 | [61 , 116] |
| 2424 | CCC(=O)c1ccccc1 | ClC(Cl)(Cl)Cl | 0.68 | 0.13 | 0.10 | 0.38 | | | | | 0.43 | [61 , 116] |
| 2425 | CCC(=O)c1ccccc1 | CCBr | -0.42 | -0.19 | -0.16 | 0.17 | | | | | 0.09 | [61 , 116] |
| 2426 | CCC(=O)c1ccccc1 | CC#N | 0.62 | 0.28 | 0.36 | 0.15 | | | | | 0.59 | [116] |
| 2427 | CCC(=O)c1ccccc1 | CI | -0.51 | -0.08 | 0.10 | 0.13 | | | | | 0.19 | [116] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2428 | CCC(=O)c1ccccc1 | CCI | -0.46 | 0.06 | 0.11 | 0.18 | | | | | 0.30 | [61 , 116] |
| 2429 | CCCOC(=O)C | C1CCCCC1 | 0.81 | 0.62 | 0.54 | 0.82 | 0.64 | 0.33 | -0.17 | 1.26 | 0.94 | [189] |
| 2430 | CCCOC(=O)C | CCCCCCC | 1.07 | 0.73 | 0.73 | 0.84 | 0.97 | 0.54 | 0.11 | 1.37 | 1.08 | [189] |
| 2431 | CCCOC(=O)C | CCCCC=C | 0.51 | 0.36 | 0.35 | 0.44 | 0.69 | 0.36 | 0.22 | 0.97 | 0.49 | [189] |
| 2432 | CCCOC(=O)C | CCCCCC | 0.96 | 0.65 | 0.65 | 0.74 | 0.85 | 0.44 | 0.18 | 1.19 | 0.92 | [119] |
| 2433 | CCCOC(=O)C | CCCCC#C | -0.22 | -0.13 | -0.13 | 0.05 | | | | | -0.05 | [190] |
| 2434 | CCCOC(=O)C | CCCC#CC | 0.14 | 0.03 | 0.02 | 0.20 | | | | | 0.09 | [190] |
| 2435 | CCCOC(=O)C | CCC#CCC | 0.17 | 0.03 | 0.02 | 0.20 | | | | | 0.21 | [190] |
| 2436 | O=[S]1(=O)CC(CC1)OCCC | CCCCCC | 2.87 | 2.45 | 2.46 | 2.46 | | | | | 2.77 | [47 , 73] |
| 2437 | O=[S]1(=O)CC(CC1)OCCC | c1ccccc1 | 0.64 | 0.39 | 0.41 | 0.28 | | | | | 0.34 | [47 , 73] |
| 2438 | CCCN | CCCCCCC | 1.34 | 0.89 | 0.98 | 1.00 | | 0.88 | 0.52 | | 1.01 | [137] |
| 2439 | CC1COC(=O)O1 | CCCCCC | 3.54 | | | | 3.68 | 3.41 | 5.08 | | 3.83 | [73 , 54 , 47] |
| 2440 | CC1COC(=O)O1 | c1ccccc1 | 1.21 | | | | 1.28 | 1.64 | 2.41 | | 1.19 | [73 , 47] |
| 2441 | CC1COC(=O)O1 | CCCCC | 3.09 | | | | 3.30 | 3.09 | 5.40 | | 3.25 | [54] |
| 2442 | CC1COC(=O)O1 | C1CCCCC1 | 3.03 | | | | 3.33 | 2.35 | 3.57 | | 3.23 | [54 , 47] |
| 2443 | CC1COC(=O)O1 | CCCC(C)C | 3.43 | | | | 3.62 | | | | 3.60 | [54] |
| 2444 | CC1COC(=O)O1 | CCCCCCC | 3.98 | | | | 4.04 | 3.72 | 4.77 | | 4.17 | [54] |
| 2445 | CC1COC(=O)O1 | CC(C)CC(C)C | 3.73 | | | | 3.88 | | | | 3.98 | [54] |
| 2446 | CC1COC(=O)O1 | CCCCCCCC | 4.42 | | | | 4.46 | 4.07 | 4.62 | | 4.60 | [54] |
| 2447 | CC1COC(=O)O1 | CC(C)C(C)C(C)C | 3.95 | | | | 4.06 | | | | 4.16 | [54] |
| 2448 | CC1COC(=O)O1 | CC(C)CCC(C)C | 4.21 | | | | | | | | 4.42 | [54] |
| 2449 | CC1COC(=O)O1 | CCC1CCCCC1 | 3.82 | | | | | | | | 3.99 | [54] |
| 2450 | CC1COC(=O)O1 | CCCCCCCCC | 4.85 | | | | 4.96 | 4.42 | 4.47 | | 5.02 | [54] |
| 2451 | CC1COC(=O)O1 | CC=C(C)C | 2.23 | | | | | 2.34 | 5.00 | | 2.61 | [47] |
| 2452 | CC1COC(=O)O1 | CC(=C)C=C | 1.41 | | | | 2.15 | | | | 1.86 | [47] |
| 2453 | CC(CO)O | Cc1ccccc1 | 2.32 | 2.26 | 1.63 | 2.73 | | 3.25 | 1.61 | | 3.27 | [191] |
| 2454 | Cc1ccc(C)cc1 | CCCCC | 0.39 | 0.29 | 0.17 | 0.47 | 0.40 | 0.13 | 0.36 | 0.41 | 0.36 | [54 , 61 , 61] |
| 2455 | Cc1ccc(C)cc1 | CCCCCC | 0.43 | 0.34 | 0.20 | 0.42 | 0.43 | 0.14 | 0.27 | 0.41 | 0.39 | [54 , 61 , 61] |
| 2456 | Cc1ccc(C)cc1 | C1CCCCC1 | 0.31 | 0.18 | 0.17 | 0.37 | 0.22 | -0.15 | -0.16 | 0.26 | 0.33 | [54 , 61 , 61] |
| 2457 | Cc1ccc(C)cc1 | CCCC(C)C | 0.41 | 0.33 | 0.20 | 0.42 | 0.49 | | | 0.49 | 0.30 | [54 , 61 , 61 , 61] |
| 2458 | Cc1ccc(C)cc1 | CCCCCCC | 0.46 | 0.36 | 0.22 | 0.37 | 0.47 | 0.13 | 0.18 | 0.42 | 0.39 | [54 , 61 , 61 , 108] |
| 2459 | Cc1ccc(C)cc1 | CC(C)CC(C)C | 0.43 | 0.35 | 0.22 | 0.37 | 0.54 | | | 0.57 | 0.38 | [54 , 61 , 61 , 61] |
| 2460 | Cc1ccc(C)cc1 | CCCCCCCC | 0.48 | 0.36 | 0.24 | 0.32 | 0.54 | 0.15 | 0.15 | 0.43 | 0.39 | [54 , 61 , 61 , 61] |
| 2461 | Cc1ccc(C)cc1 | CC(C)C(C)C(C)C | 0.42 | 0.35 | 0.24 | 0.32 | 0.28 | | | | 0.44 | [54 , 61 , 61] |
| 2462 | Cc1ccc(C)cc1 | CC(C)CCC(C)C | 0.48 | 0.36 | 0.24 | 0.32 | | | | | 0.51 | [54] |
| 2463 | Cc1ccc(C)cc1 | CCC1CCCCC1 | 0.37 | 0.24 | 0.22 | 0.29 | | | | 0.37 | 0.35 | [54 , 61 , 61] |
| 2464 | Cc1ccc(C)cc1 | CCCCCCCCC | 0.51 | 0.35 | 0.25 | 0.27 | 0.70 | 0.16 | 0.12 | 0.43 | 0.39 | [54 , 61 , 61 , 61] |
| 2465 | Cc1ccc(C)cc1 | c1ccccc1 | -0.06 | -0.12 | -0.08 | 0.02 | 0.06 | -0.26 | -0.27 | -0.04 | 0.03 | [61 , 192] |
| 2466 | Cc1ccc(C)cc1 | Cc1ccccc1 | 0.00 | -0.02 | -0.02 | 0.00 | 0.00 | -0.22 | -0.22 | -0.01 | -0.03 | [61] |
| 2467 | Cc1ccc(C)cc1 | CCCC=C | 0.17 | 0.03 | -0.08 | 0.36 | 0.36 | 0.14 | 0.36 | 0.25 | 0.22 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2468 | Cc1ccc(C)cc1 | CC(C)C=C | 0.18 | 0.03 | -0.08 | 0.36 | | | | | 0.17 | [61] |
| 2469 | Cc1ccc(C)cc1 | CC(=C)C=C | 0.03 | -0.09 | -0.15 | 0.21 | 0.25 | | | | 0.03 | [61] |
| 2470 | Cc1ccc(C)cc1 | CCO | 3.48 | 2.26 | 1.87 | 2.82 | 2.94 | 0.75 | 3.22 | 3.56 | 2.75 | [61] |
| 2471 | Cc1ccc(C)cc1 | CCOC(=O)C | 0.39 | 0.11 | -0.07 | 0.46 | 0.63 | 0.05 | -0.29 | 0.55 | 0.28 | [61] |
| 2472 | Cc1ccc(C)cc1 | C1COCCO1 | 0.30 | 1.28 | 0.63 | -0.06 | 0.12 | -0.16 | 0.03 | 0.23 | 0.22 | [61] |
| 2473 | Cc1ccc(C)cc1 | CC(C)=O | 0.90 | 0.30 | 0.20 | 0.77 | 1.02 | 0.18 | -0.15 | 0.62 | 0.74 | [61] |
| 2474 | Cc1ccc(C)cc1 | CCC(C)=O | 0.66 | 0.17 | 0.04 | 0.59 | 0.63 | 0.14 | -0.22 | 0.30 | 0.35 | [61] |
| 2475 | Cc1ccc(C)cc1 | CCCCl | 0.15 | -0.19 | -0.27 | -0.03 | 0.10 | | | | 0.03 | [61] |
| 2476 | Cc1ccc(C)cc1 | CC(C)(C)Cl | 0.29 | 0.04 | -0.13 | 0.09 | 0.19 | | | | 0.22 | [61] |
| 2477 | Cc1ccc(C)cc1 | ClCCl | 0.10 | -0.25 | -0.25 | -0.16 | -0.06 | -0.26 | -0.15 | -0.12 | -0.16 | [61] |
| 2478 | Cc1ccc(C)cc1 | ClC(Cl)(Cl)Cl | 0.36 | -0.11 | -0.19 | -0.11 | -0.04 | -0.21 | -0.26 | -0.07 | -0.07 | [61] |
| 2479 | Cc1ccc(C)cc1 | CCBr | -0.02 | 0.51 | 0.48 | -0.12 | 0.09 | -0.08 | | | 0.00 | [61] |
| 2480 | Cc1ccc(C)cc1 | CCI | -0.07 | 0.02 | 0.02 | 0.10 | 0.44 | | | | 0.03 | [61] |
| 2481 | Cc1ccc(C)cc1 | CCN(CC)CC | 0.25 | 0.13 | 0.00 | 0.09 | 0.31 | -0.12 | -0.16 | 0.17 | 0.08 | [61] |
| 2482 | Cc1ccc(C)cc1 | C(=S)=S | 0.00 | 0.00 | 0.12 | 0.09 | | -0.29 | -0.11 | | 0.07 | [61] |
| 2483 | c1ccncc1 | CCCCCC | 1.74 | 1.33 | 1.03 | 1.99 | 1.82 | 1.32 | 1.49 | 1.93 | 1.81 | [47 , 54 , 61 , 73] |
| 2484 | c1ccncc1 | c1ccccc1 | 0.22 | 0.25 | 0.22 | 0.12 | 0.47 | 0.34 | 0.21 | 0.37 | 0.18 | [47 , 73] |
| 2485 | c1ccncc1 | CCCCC | 1.55 | 1.22 | 0.91 | 1.94 | 1.70 | 1.23 | 1.66 | 1.83 | 1.70 | [54 , 61 , 74] |
| 2486 | c1ccncc1 | C1CCCCC1 | 1.41 | 0.98 | 0.88 | | 1.59 | 0.72 | 0.71 | 1.56 | 1.47 | [54 , 61 , 193] |
| 2487 | c1ccncc1 | CCCC(C)C | 1.69 | 1.32 | 1.03 | 1.99 | 1.85 | | | 2.04 | 1.84 | [54 , 61] |
| 2488 | c1ccncc1 | CCCCCCC | 1.92 | 1.41 | 1.15 | 2.03 | 1.93 | 1.40 | 1.33 | 2.06 | 1.94 | [54 , 61 , 194] |
| 2489 | c1ccncc1 | CC(C)CC(C)C | 1.81 | 1.40 | 1.15 | 2.03 | 1.95 | | | 2.26 | 2.01 | [54 , 61] |
| 2490 | c1ccncc1 | CCCCCCCC | 2.09 | 1.47 | 1.26 | 2.07 | 2.09 | 1.52 | 1.26 | 2.18 | 2.11 | [54 , 61 , 61 , 194] |
| 2491 | c1ccncc1 | CC(C)C(C)C(C)C | 1.86 | 1.46 | 1.26 | 2.07 | 1.80 | | | | 2.01 | [54 , 61] |
| 2492 | c1ccncc1 | CC(C)CCC(C)C | 2.02 | 1.46 | 1.26 | 2.07 | | | | | 2.11 | [54] |
| 2493 | c1ccncc1 | CCC1CCCCC1 | 1.74 | 1.16 | 1.12 | | | | | 1.95 | 1.80 | [54] |
| 2494 | c1ccncc1 | CCCCCCCCC | 2.26 | 1.52 | 1.36 | 2.12 | 2.33 | 1.62 | 1.19 | 2.31 | 2.22 | [54 , 194] |
| 2495 | c1ccncc1 | CCC(C)CCC(C)C | 2.14 | 1.52 | 1.36 | 2.12 | | | | | 2.05 | [61] |
| 2496 | c1ccncc1 | CCCCCCCCCC | 2.43 | 1.57 | 1.47 | 2.16 | 2.54 | 1.78 | 1.19 | 2.43 | 2.26 | [194] |
| 2497 | c1ccncc1 | CCCCCCCCCCC | 2.58 | 1.60 | 1.57 | 2.20 | 2.31 | | | | 2.32 | [194] |
| 2498 | c1ccncc1 | Cc1ccccc1 | 0.41 | 0.55 | 0.53 | 0.42 | 0.49 | 0.34 | 0.32 | 0.52 | 0.35 | [61] |
| 2499 | c1ccncc1 | Cc1cccc(C)c1 | 0.54 | 0.78 | 0.80 | 0.74 | 0.64 | 0.45 | 0.36 | | 0.43 | [194] |
| 2500 | c1ccncc1 | Cc1ccc(C)cc1 | 0.55 | 0.78 | 0.80 | 0.74 | 0.57 | 0.46 | 0.41 | 0.75 | 0.44 | [194] |
| 2501 | c1ccncc1 | Cc1ccccc1C | 0.45 | 0.78 | 0.80 | 0.74 | 0.52 | 0.43 | 0.36 | | 0.34 | [194] |
| 2502 | c1ccncc1 | CCc1ccccc1 | 0.54 | 0.55 | 0.56 | 0.73 | 0.67 | 0.58 | 0.42 | 0.73 | 0.36 | [194] |
| 2503 | c1ccncc1 | CCCC=C | 0.96 | 1.24 | 0.95 | 1.76 | 1.50 | 0.95 | 1.66 | 1.45 | 1.36 | [74] |
| 2504 | c1ccncc1 | C1CCC=CC1 | 0.88 | 0.97 | 0.88 | | 1.21 | 0.31 | 0.36 | | 0.91 | [194] |
| 2505 | c1ccncc1 | CCCCCC=C | 1.29 | 1.42 | 1.18 | 1.88 | 1.63 | 1.05 | 1.34 | | 1.27 | [194] |
| 2506 | c1ccncc1 | CCCCCC#C | 0.55 | -0.22 | -0.43 | 1.41 | | | | | 0.44 | [194] |
| 2507 | c1ccncc1 | CCO | -0.37 | -0.07 | -0.80 | -0.25 | 0.02 | 0.50 | 0.41 | -0.05 | -0.22 | [61] |
| 2508 | c1ccncc1 | CCCCOC(=O)C | 0.27 | 0.03 | -0.33 | 0.20 | 0.26 | 0.44 | 0.56 | 0.58 | 0.14 | [194] |
| 2509 | c1ccncc1 | CCCCCOC(=O)C | 0.36 | 0.01 | -0.30 | 0.16 | | | | | 0.11 | [194] |
| 2510 | c1ccncc1 | C1CCOC1 | 0.12 | 0.32 | -0.13 | | -0.16 | -0.03 | 0.00 | 0.22 | -0.07 | [194] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2511 | c1ccncc1 | C1COCCO1 | 0.07 | 0.67 | -0.37 | | -0.25 | 0.09 | -0.12 | 0.20 | -0.04 | [61] |
| 2512 | c1ccncc1 | CC(C)=O | 0.20 | 0.20 | -0.14 | 0.19 | 0.15 | 0.02 | -0.09 | 0.36 | 0.17 | [194] |
| 2513 | c1ccncc1 | CCC(C)=O | 0.15 | 0.13 | -0.22 | 0.10 | 0.19 | 0.03 | 0.10 | 0.34 | -0.03 | [61] |
| 2514 | c1ccncc1 | CCCCCl | 0.43 | 0.51 | 0.22 | 0.22 | 0.55 | 0.20 | 0.51 | 0.75 | 0.43 | [194] |
| 2515 | c1ccncc1 | CC(Cl)CCl | -0.07 | 0.22 | -0.02 | -0.78 | 0.15 | | | | -0.07 | [194] |
| 2516 | c1ccncc1 | CC(C)Br | -0.27 | -0.12 | -0.39 | 0.39 | | | | | 0.30 | [194] |
| 2517 | c1ccncc1 | CC#N | 0.51 | -0.16 | -0.40 | 0.43 | -0.13 | 0.12 | -0.12 | 0.24 | 0.38 | [194] |
| 2518 | C1CCNC1 | C1CCCCC1 | 0.82 | 0.45 | 0.46 | 0.69 | | 0.51 | 5.72 | | 0.90 | [160] |
| 2519 | c1ccc2ncccc2c1 | CCCCC | 1.41 | 1.15 | 0.59 | 1.89 | | 1.03 | 2.55 | 1.93 | 1.44 | [195 , 195] |
| 2520 | c1ccc2ncccc2c1 | C1CCCC1 | 1.08 | 0.68 | 0.46 | | | 0.27 | 1.24 | 1.31 | 0.80 | [195 , 195 , 195] |
| 2521 | c1ccc2ncccc2c1 | CCCCCC | 1.60 | 1.31 | 0.69 | 1.99 | | 1.10 | 2.30 | 2.10 | 1.71 | [195 , 195 , 61 , 116] |
| 2522 | c1ccc2ncccc2c1 | C1CCCCC1 | 1.24 | 0.86 | 0.58 | | | 0.43 | 1.12 | 1.54 | 1.25 | [195 , 195 , 195 , 61 , 116] |
| 2523 | c1ccc2ncccc2c1 | CCCCCCC | 1.78 | 1.45 | 0.79 | 2.09 | | 1.14 | 2.06 | 2.28 | 1.58 | [195 , 195] |
| 2524 | c1ccc2ncccc2c1 | c1ccccc1 | 0.15 | 0.09 | 0.02 | 0.27 | | 0.01 | 0.34 | 0.30 | 0.15 | [195 , 195 , 61 , 116] |
| 2525 | c1ccc2ncccc2c1 | C1C=CC=C1 | 0.22 | 0.55 | 0.45 | | | | | | 1.03 | [61 , 116] |
| 2526 | c1ccc2ncccc2c1 | CC(=C)C=C | 0.54 | 0.93 | 0.52 | 0.75 | | | | | 0.89 | [61 , 116] |
| 2527 | c1ccc2ncccc2c1 | CO | -0.11 | -0.39 | -0.67 | 0.59 | | 0.38 | 2.07 | 0.76 | -0.27 | [195 , 195 , 195] |
| 2528 | c1ccc2ncccc2c1 | CCOC(=O)C | 0.19 | 0.36 | -0.29 | 0.55 | | 0.08 | 0.24 | 0.38 | 0.40 | [61 , 116] |
| 2529 | c1ccc2ncccc2c1 | CC(C)=O | 0.32 | 0.40 | -0.06 | 0.48 | | 0.10 | -0.12 | 0.25 | 0.41 | [61 , 116] |
| 2530 | c1ccc2ncccc2c1 | CCCCl | 0.30 | 0.31 | -0.12 | 0.62 | | | | | 0.26 | [61 , 116] |
| 2531 | c1ccc2ncccc2c1 | CC(C)(C)Cl | 0.43 | 0.81 | 0.19 | 1.11 | | | | | 0.52 | [61 , 116] |
| 2532 | c1ccc2ncccc2c1 | ClCCCl | -0.11 | 0.20 | -0.16 | 0.03 | | -0.27 | -0.24 | -0.19 | -0.08 | [116] |
| 2533 | c1ccc2ncccc2c1 | ClC(Cl)Cl | -0.69 | -0.42 | -0.69 | -0.89 | | -0.20 | | -0.82 | -0.76 | [61 , 116] |
| 2534 | c1ccc2ncccc2c1 | ClC(Cl)(Cl)Cl | 0.48 | 0.19 | -0.25 | 0.41 | | 0.18 | 0.63 | 0.59 | 0.36 | [61 , 116] |
| 2535 | c1ccc2ncccc2c1 | CCBr | -0.39 | -0.22 | -0.56 | 0.59 | | -0.06 | | | 0.24 | [61 , 116] |
| 2536 | c1ccc2ncccc2c1 | CC#N | 0.70 | 0.10 | -0.16 | 0.59 | | 0.26 | -0.24 | 0.25 | 0.76 | [116] |
| 2537 | c1ccc2ncccc2c1 | CI | -0.60 | -0.25 | -0.21 | -0.01 | | | | 0.31 | 0.22 | [116] |
| 2538 | c1ccc2ncccc2c1 | CCI | -0.49 | -0.01 | -0.27 | 0.31 | | | | | 0.44 | [61 , 116] |
| 2539 | c1ccc2ncccc2c1 | CCN(CC)CC | 1.05 | 0.81 | 0.17 | 1.69 | | 0.39 | 0.71 | 1.43 | 0.19 | [116] |
| 2540 | CCC(C)N | CCCCCCC | 1.05 | 0.46 | 0.49 | 0.72 | | | | | 0.77 | [137] |
| 2541 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCC | -0.34 | -0.84 | -0.45 | -0.39 | | | | -0.73 | -0.48 | [97 , 61] |
| 2542 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | C1CCCC1 | -0.42 | -0.97 | -0.51 | -0.49 | | | | -0.71 | -0.73 | [97 , 61] |
| 2543 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(C)C | -0.34 | -0.84 | -0.45 | -0.39 | | | | | -0.46 | [97] |
| 2544 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCC | -0.29 | -0.71 | -0.39 | -0.33 | | | | -0.63 | -0.44 | [97 , 61 , 54] |
| 2545 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | C1CCCCC1 | -0.36 | -0.82 | -0.43 | -0.40 | | | | -0.54 | -0.65 | [97 , 61 , 61] |
| 2546 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCC(C)C | -0.30 | -0.71 | -0.39 | -0.33 | | | | -0.63 | -0.40 | [97] |
| 2547 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(C)CC | -0.30 | -0.71 | -0.39 | -0.33 | | | | | -0.45 | [97] |
| 2548 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC1CCCC1 | -0.34 | -0.82 | -0.43 | -0.48 | | | | -0.63 | -0.60 | [97] |
| 2549 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)C(C)C | -0.30 | -0.71 | -0.39 | -0.33 | | | | -0.63 | -0.45 | [97] |
| 2550 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(C)(C)C | -0.30 | -0.69 | -0.39 | -0.33 | | | | | -0.46 | [97 , 196 , 196] |

Continued on next page

**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2551 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCCC | -0.25 | -0.62 | -0.31 | -0.29 | | | | -0.53 | -0.38 | [97 , 61 , 61] |
| 2552 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCC(C)CC | -0.26 | -0.62 | -0.31 | -0.29 | | | | | -0.36 | [97] |
| 2553 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCC(C)(C)C | -0.25 | -0.60 | -0.31 | -0.29 | | | | | -0.34 | [97] |
| 2554 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)CC(C)C | -0.25 | -0.62 | -0.31 | -0.29 | | | | -0.54 | -0.33 | [97] |
| 2555 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(CC)CC | -0.26 | -0.62 | -0.31 | -0.29 | | | | | -0.43 | [97] |
| 2556 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC1CCCCC1 | -0.30 | -0.71 | -0.36 | -0.37 | | | | -0.53 | -0.63 | [97 , 61 , 61] |
| 2557 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCCCC | -0.21 | -0.53 | -0.27 | -0.25 | | | | -0.43 | -0.34 | [97 , 61] |
| 2558 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)CC(C)(C)C | -0.21 | -0.51 | -0.27 | -0.25 | | | | -0.46 | -0.33 | [97] |
| 2559 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC1CCCCC1 | -0.26 | -0.60 | -0.30 | -0.33 | | | | -0.37 | -0.58 | [97] |
| 2560 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCCCCC | -0.19 | -0.46 | -0.24 | -0.22 | | | | -0.34 | -0.29 | [97] |
| 2561 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | c1ccccc1 | 0.03 | -0.58 | -0.13 | -0.29 | | | | -0.24 | -0.35 | [97 , 61 , 61] |
| 2562 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | Cc1ccccc1 | 0.08 | -0.45 | -0.06 | -0.30 | | | | -0.17 | -0.34 | [97 , 61 , 61] |
| 2563 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | Cc1cccc(C)c1 | 0.05 | -0.36 | -0.05 | -0.31 | | | | | -0.27 | [97] |
| 2564 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | Cc1ccc(C)cc1 | 0.04 | -0.36 | -0.05 | -0.31 | | | | -0.24 | -0.29 | [97] |
| 2565 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | Cc1ccccc1C | 0.07 | -0.36 | -0.05 | -0.31 | | | | | -0.27 | [97] |
| 2566 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCc1ccccc1 | 0.10 | -0.40 | -0.07 | -0.25 | | | | -0.05 | -0.25 | [97] |
| 2567 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCC=C | -0.33 | -0.82 | -0.40 | -0.45 | | | | -0.76 | -0.48 | [97] |
| 2568 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(C)C=C | -0.27 | -0.69 | -0.33 | -0.39 | | | | | -0.48 | [97] |
| 2569 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCC=C | -0.27 | -0.69 | -0.33 | -0.39 | | | | -0.63 | -0.45 | [97] |
| 2570 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | C1CCC=CC1 | -0.34 | -0.82 | -0.40 | -0.49 | | | | | -0.65 | [97] |
| 2571 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCC=C | -0.24 | -0.60 | -0.27 | -0.33 | | | | | -0.40 | [97] |
| 2572 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCCCC=C | -0.21 | -0.51 | -0.24 | -0.27 | | | | -0.48 | -0.34 | [97] |
| 2573 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CO | 3.91 | 1.83 | 2.48 | 3.39 | | | | 5.07 | 3.66 | [61] |
| 2574 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCO | 3.75 | 2.36 | 2.66 | 3.03 | | | | 2.03 | 3.26 | [61] |
| 2575 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCO | 3.72 | 2.26 | 2.53 | 2.92 | | | | 2.81 | 3.04 | [61] |
| 2576 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)O | 3.27 | 2.26 | 2.53 | 2.73 | | | | 2.58 | 2.83 | [61] |
| 2577 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCCCO | 3.44 | 2.17 | 2.42 | 2.84 | | | | 2.98 | 3.03 | [61] |
| 2578 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)CO | 3.18 | 2.17 | 2.42 | 2.84 | | | | 2.81 | 2.88 | [61] |
| 2579 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(=O)OC | 1.01 | 0.31 | 0.76 | 0.85 | | | | 0.72 | 0.83 | [61] |
| 2580 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCOC(=O)C | 0.82 | 0.27 | 0.66 | 0.74 | | | | 0.72 | 0.67 | [61] |
| 2581 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | C1CCOC1 | 0.03 | -0.34 | 0.01 | -0.20 | | | | -0.31 | -0.26 | [61] |
| 2582 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCOCC | -0.12 | -0.63 | -0.24 | -0.24 | | | | -0.48 | -0.27 | [61] |
| 2583 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC(C)=O | 1.51 | 0.81 | 1.31 | 1.04 | | | | 0.84 | 1.28 | [61] |
| 2584 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CCC(C)=O | 1.17 | 0.77 | 1.19 | 0.96 | | | | 0.61 | 0.94 | [61] |
| 2585 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | ClC(Cl)(Cl)Cl | -0.29 | -0.80 | -0.36 | -0.49 | | | | -0.53 | -0.33 | [61] |
| 2586 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | CC#N | 3.11 | 2.16 | 2.79 | 2.45 | | | | | 2.84 | [61] |
| 2587 | O=[S](=O)NCCCCCC | CCCCCC | 5.91 | 4.07 | 4.05 | 5.69 | | | | | 5.68 | [73] |
| 2588 | O=[S](=O)NCCCCC | c1ccccc1 | 2.40 | 1.02 | 1.03 | 1.63 | | | | | 2.15 | [73] |
| 2589 | O=[S]1(=O)CCCC1 | CCCCCC | 4.22 | 3.38 | 3.33 | 3.93 | | 4.36 | 7.92 | 4.11 | 4.22 | [73 , 47 , 84] |
| 2590 | O=[S]1(=O)CCCC1 | c1ccccc1 | 1.34 | 0.78 | 0.77 | 0.88 | | 2.07 | 4.32 | 1.01 | 0.88 | [73 , 47 , 84] |
| 2591 | O=[S]1(=O)CCCC1 | C1CCCCC1 | 3.59 | 2.80 | 2.80 | 3.39 | | 3.07 | 5.91 | 3.32 | 3.51 | [84] |
| 2592 | O=[S]1(=O)CCCC1 | CC1CCCC1 | 3.63 | 2.79 | 2.79 | 3.05 | | | | 3.45 | 3.54 | [84] |
| 2593 | O=[S]1(=O)CCCC1 | CCCCCCC | 4.75 | 3.81 | 3.78 | 4.33 | | 4.77 | 7.50 | 4.52 | 4.37 | [84] |
| 2594 | O=[S]1(=O)CCCC1 | CC1CCCCC1 | 4.05 | 3.25 | 3.25 | 3.61 | | 3.75 | 6.71 | 3.89 | 3.86 | [84] |
| 2595 | O=[S]1(=O)CCCC1 | CC(C)CC(C)(C)C | 4.77 | 4.32 | 4.29 | 4.73 | | 5.94 | 8.87 | 5.31 | 4.36 | [84] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2596 | O=[S]1(=O)CCCC1 | Cc1ccccc1 | 1.86 | 1.34 | 1.32 | 1.29 | | 2.29 | 4.66 | 1.46 | 1.34 | [84] |
| 2597 | NC1CCC[S]1(=O)=O | CCCCCC | 5.91 | 4.07 | 4.05 | 5.69 | | | | | 5.68 | [73] |
| 2598 | NC1CCC[S]1(=O)=O | c1ccccc1 | 2.40 | 1.02 | 1.03 | 1.63 | | | | | 2.15 | [73] |
| 2599 | C1C=CCS1(=O)=O | CCCCCC | 4.70 | 3.70 | 3.64 | 5.54 | | | | | 4.61 | [47 , 73] |
| 2600 | C1C=CCS1(=O)=O | c1ccccc1 | 1.63 | 0.75 | 0.74 | 1.53 | | | | | 0.79 | [47 , 73] |
| 2601 | CCC(C)(C)OC | CCCCCC | 0.22 | 0.32 | 0.31 | 0.19 | | | | | 0.22 | [197] |
| 2602 | CCC(C)(C)OC | CCC(C)(C)C | 0.18 | 0.32 | 0.32 | 0.19 | | | | | 0.18 | [198] |
| 2603 | CCC(C)(C)OC | CCCCCCCC | 0.28 | 0.41 | 0.40 | 0.23 | | | | | 0.36 | [132] |
| 2604 | ClC(Cl)(Cl)Cl | CCCCC | 0.32 | 0.10 | 0.10 | 0.32 | 0.10 | 0.15 | 0.22 | 0.41 | 0.26 | [54 , 61 , 61] |
| 2605 | ClC(Cl)(Cl)Cl | C1CCCC1 | 0.21 | 0.12 | 0.09 | 0.10 | -0.06 | -0.15 | -0.15 | 0.16 | 0.05 | [125] |
| 2606 | ClC(Cl)(Cl)Cl | CCCCCC | 0.31 | 0.08 | 0.10 | 0.29 | 0.07 | 0.14 | 0.16 | 0.35 | 0.27 | [54 , 61 , 61] |
| 2607 | ClC(Cl)(Cl)Cl | C1CCCCC1 | 0.17 | 0.13 | 0.10 | 0.09 | -0.02 | -0.14 | -0.14 | 0.20 | 0.07 | [54 , 61 , 61 , 125] |
| 2608 | ClC(Cl)(Cl)Cl | CCCC(C)C | 0.31 | 0.08 | 0.10 | 0.29 | 0.15 | | | 0.45 | 0.31 | [54 , 61 , 61] |
| 2609 | ClC(Cl)(Cl)Cl | CCCCCCC | 0.30 | 0.04 | 0.10 | 0.25 | 0.04 | 0.11 | 0.10 | 0.30 | 0.29 | [54] |
| 2610 | ClC(Cl)(Cl)Cl | CC(C)CC(C)C | 0.31 | 0.04 | 0.10 | 0.25 | 0.16 | | | 0.49 | 0.34 | [54 , 61 , 61] |
| 2611 | ClC(Cl)(Cl)Cl | C1CCCCC1 | 0.10 | 0.10 | 0.10 | 0.05 | -0.30 | | | 0.23 | 0.13 | [125] |
| 2612 | ClC(Cl)(Cl)Cl | CCCCCCCC | 0.28 | -0.02 | 0.09 | 0.22 | 0.05 | 0.11 | 0.08 | 0.25 | 0.25 | [54 , 61 , 61 , 61] |
| 2613 | ClC(Cl)(Cl)Cl | C1CCCCCCC1 | 0.08 | 0.07 | 0.09 | 0.01 | -0.42 | -0.12 | -0.13 | 0.25 | 0.15 | [125] |
| 2614 | ClC(Cl)(Cl)Cl | CC(C)C(C)C(C)C | 0.27 | -0.02 | 0.09 | 0.22 | -0.20 | | | | 0.28 | [54 , 61 , 61] |
| 2615 | ClC(Cl)(Cl)Cl | CC(C)CCC(C)C | 0.30 | -0.02 | 0.09 | 0.22 | | | | | 0.32 | [54] |
| 2616 | ClC(Cl)(Cl)Cl | CCC1CCCCC1 | 0.17 | 0.07 | 0.09 | 0.08 | | | | 0.20 | 0.19 | [54 , 61 , 61] |
| 2617 | ClC(Cl)(Cl)Cl | CCCCCCCCC | 0.25 | -0.08 | 0.07 | 0.18 | 0.14 | 0.11 | 0.06 | 0.20 | 0.26 | [54 , 61 , 61] |
| 2618 | ClC(Cl)(Cl)Cl | CCC(C)CCC(C)C | 0.25 | -0.08 | 0.07 | 0.18 | | | | | 0.24 | [61] |
| 2619 | ClC(Cl)(Cl)Cl | C1CCCCCCCC1 | 0.03 | -0.06 | 0.05 | -0.09 | | | | | 0.17 | [125] |
| 2620 | ClC(Cl)(Cl)Cl | c1ccccc1 | 0.53 | 0.10 | -0.01 | 0.12 | 0.19 | -0.20 | -0.19 | 0.07 | 0.06 | [61 , 61] |
| 2621 | ClC(Cl)(Cl)Cl | Cc1ccccc1 | 0.54 | 0.00 | -0.12 | 0.02 | 0.06 | -0.15 | -0.16 | 0.04 | 0.02 | [61] |
| 2622 | ClC(Cl)(Cl)Cl | CC(=C)C=C | 0.55 | 0.12 | 0.12 | 0.22 | 0.20 | | | | 0.00 | [61] |
| 2623 | ClC(Cl)(Cl)Cl | CCO | 4.03 | 2.90 | 2.77 | 3.52 | 3.63 | 1.22 | 2.76 | 3.82 | 3.33 | [61] |
| 2624 | ClC(Cl)(Cl)Cl | CCCO | 3.94 | 2.65 | 2.56 | 3.32 | 3.32 | 1.28 | 1.65 | 3.53 | 3.16 | [61] |
| 2625 | ClC(Cl)(Cl)Cl | CCCCO | 3.60 | 2.43 | 2.37 | 3.15 | 3.05 | 1.32 | 1.02 | 3.18 | 2.80 | [61] |
| 2626 | ClC(Cl)(Cl)Cl | CCC(C)O | 3.17 | 2.43 | 2.37 | 2.97 | 2.87 | 1.13 | 0.62 | 2.83 | 2.67 | [61] |
| 2627 | ClC(Cl)(Cl)Cl | CC(C)CO | 3.37 | 2.43 | 2.37 | 3.15 | 3.11 | 1.45 | 0.80 | 3.11 | 2.87 | [61] |
| 2628 | ClC(Cl)(Cl)Cl | CC(C)(C)O | 3.31 | 2.02 | 2.04 | 2.53 | | 1.25 | 0.48 | 2.39 | 2.75 | [61] |
| 2629 | ClC(Cl)(Cl)Cl | C1COCCO1 | 0.82 | 0.80 | 0.55 | -0.08 | 0.29 | 0.06 | 0.10 | 0.29 | 0.22 | [61] |
| 2630 | ClC(Cl)(Cl)Cl | CC(C)=O | 1.59 | 1.10 | 1.10 | 1.06 | 1.34 | 0.48 | -0.06 | 0.93 | 1.14 | [61] |
| 2631 | ClC(Cl)(Cl)Cl | CCC(C)=O | 1.23 | 0.91 | 0.90 | 0.89 | 0.81 | 0.41 | -0.13 | 0.44 | 0.78 | [61] |
| 2632 | ClC(Cl)(Cl)Cl | O=C1CCC1 | 1.22 | 0.59 | 0.57 | 0.63 | | 0.41 | 0.55 | | 1.06 | [71] |
| 2633 | ClC(Cl)(Cl)Cl | CCCCC=O | 0.81 | -1.56 | -1.56 | -1.35 | | 0.68 | -0.07 | | 0.53 | [71] |
| 2634 | ClC(Cl)(Cl)Cl | CCCCl | 0.45 | 0.07 | 0.07 | 0.21 | 0.11 | | | | 0.23 | [61] |
| 2635 | ClC(Cl)(Cl)Cl | ClCCl | 0.55 | 0.39 | 0.43 | 0.44 | 0.29 | -0.05 | -0.05 | 0.34 | 0.45 | [61] |
| 2636 | ClC(Cl)(Cl)Cl | ClC(Cl)Cl | 0.15 | 0.16 | 0.16 | 0.17 | 0.10 | -0.07 | | 0.10 | 0.15 | [61] |
| 2637 | ClC(Cl)(Cl)Cl | CCBr | 0.26 | 0.09 | 0.10 | 0.33 | 0.16 | 0.09 | | | 0.22 | [61] |
| 2638 | ClC(Cl)(Cl)Cl | CCC#N | 1.10 | 1.45 | 1.46 | 1.51 | 1.74 | 0.77 | 0.35 | 1.70 | 1.94 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2639 | ClC(Cl)(Cl)Cl | CC(C)[N+]([O-])=O | 1.13 | 1.14 | 1.14 | 1.36 | | 0.70 | 0.15 | | 1.61 | [61] |
| 2640 | ClC(Cl)(Cl)Cl | CCI | 0.17 | 0.29 | 0.29 | 0.23 | 0.54 | | | | 0.29 | [61] |
| 2641 | ClC(Cl)(Cl)Cl | CCN(CC)CC | 0.17 | -0.37 | -0.31 | -0.31 | 0.03 | -0.12 | -0.12 | -0.31 | -0.37 | [61] |
| 2642 | ClC(Cl)(Cl)Cl | C(=S)=S | 0.20 | 0.27 | 0.31 | 0.21 | | -0.24 | -0.01 | | 0.19 | [61] |
| 2643 | COCCOCCOCCOCCOC | CCCCC | 0.56 | 1.06 | 1.20 | 0.55 | | | | 1.25 | 1.39 | [199] |
| 2644 | COCCOCCOCCOCCOC | CCCCCC | 0.69 | 1.36 | 1.45 | 0.69 | | | | 1.42 | 1.56 | [199] |
| 2645 | COCCOCCOCCOCCOC | CCCCCCC | 0.81 | 1.64 | 1.70 | 0.83 | | | | 1.62 | 1.76 | [199] |
| 2646 | COCCOCCOCCOCCOC | CCCCCCCC | 0.92 | 1.91 | 1.93 | 0.97 | | | | 1.82 | 1.94 | [199] |
| 2647 | C1CCOC1 | CCCCC | 0.53 | 0.59 | 0.58 | 0.46 | 0.78 | 0.70 | 0.43 | 0.80 | 0.66 | [54 , 61 , 61 , 74] |
| 2648 | C1CCOC1 | CCCCCC | 0.59 | 0.65 | 0.65 | 0.47 | 0.85 | 0.78 | 0.35 | 0.80 | 0.74 | [54 , 61 , 61] |
| 2649 | C1CCOC1 | C1CCCCC1 | 0.51 | 0.70 | 0.56 | 0.44 | 0.59 | 0.48 | -0.03 | 0.72 | 0.59 | [54 , 61 , 85 , 85] |
| 2650 | C1CCOC1 | CCCC(C)C | 0.56 | 0.65 | 0.65 | 0.47 | 0.89 | | | 0.86 | 0.73 | [54 , 61 , 61] |
| 2651 | C1CCOC1 | CCCCCCC | 0.64 | 0.68 | 0.71 | 0.47 | 0.92 | 0.85 | 0.27 | 0.81 | 0.83 | [54] |
| 2652 | C1CCOC1 | CC(C)CC(C)C | 0.58 | 0.68 | 0.71 | 0.47 | 0.97 | | | 0.93 | 0.74 | [54 , 61 , 61] |
| 2653 | C1CCOC1 | CCCCCCCC | 0.68 | 0.69 | 0.77 | 0.48 | 1.03 | 0.94 | 0.24 | 0.82 | 0.75 | [54 , 61 , 61 , 61] |
| 2654 | C1CCOC1 | CC(C)C(C)C(C)C | 0.58 | 0.69 | 0.76 | 0.48 | 0.75 | | | | 0.78 | [54 , 61] |
| 2655 | C1CCOC1 | CC(C)CCC(C)C | 0.64 | 0.69 | 0.76 | 0.48 | | | | | 0.79 | [54] |
| 2656 | C1CCOC1 | CCC1CCCCC1 | 0.59 | 0.78 | 0.68 | 0.45 | | | | 0.80 | 0.73 | [54 , 61 , 61] |
| 2657 | C1CCOC1 | CCCCCCCCC | 0.72 | 0.69 | 0.82 | 0.48 | 1.22 | 1.03 | 0.22 | 0.82 | 0.84 | [54 , 61 , 61] |
| 2658 | C1CCOC1 | Cc1ccccc1 | -0.02 | 0.34 | 0.05 | -0.34 | 0.03 | 0.25 | -0.13 | -0.12 | -0.20 | [61] |
| 2659 | C1CCOC1 | CCCC=C | 0.20 | 0.44 | 0.42 | 0.26 | 0.67 | 0.33 | 0.43 | 0.55 | 0.20 | [74] |
| 2660 | C1CCOC1 | C1COCCO1 | 0.13 | 0.30 | 0.21 | 0.11 | -0.13 | 0.00 | -0.06 | 0.22 | 0.12 | [61] |
| 2661 | C1CCOC1 | CCC=O | 0.17 | 0.29 | 0.29 | -0.34 | | | | | 0.12 | [61] |
| 2662 | C1CCOC1 | CCCC=O | 0.04 | 0.21 | 0.19 | -0.43 | 0.36 | -0.07 | -0.11 | 0.13 | 0.17 | [61] |
| 2663 | C1CCOC1 | CCN(CC)CC | 0.16 | 0.48 | 0.50 | 0.40 | 0.63 | 0.59 | -0.07 | 0.51 | 0.36 | [61] |
| 2664 | C1CC(OC1)CO | CCCCCC | 2.00 | 2.37 | 2.23 | 2.13 | | 1.49 | 1.89 | | 2.71 | [47 , 47] |
| 2665 | C1CC(OC1)CO | c1ccccc1 | 0.69 | 1.16 | 0.74 | 0.65 | | 0.51 | 0.29 | | 0.79 | [73 , 73] |
| 2666 | C1CCc2ccccc2C1 | CCCCCC | 0.44 | 0.39 | 0.13 | 0.50 | | 0.59 | 0.90 | | 0.64 | [118] |
| 2667 | C1CCc2ccccc2C1 | C1CCCCC1 | 0.29 | 0.16 | 0.10 | 0.29 | | 0.02 | 0.11 | | 0.31 | [118] |
| 2668 | C1CCc2ccccc2C1 | CCCCCCC | 0.48 | 0.44 | 0.16 | 0.51 | | 0.59 | 0.75 | | 0.63 | [118] |
| 2669 | C1CCc2ccccc2C1 | c1ccccc1 | -0.11 | -0.01 | 0.04 | -0.01 | | -0.26 | -0.27 | | -0.04 | [118] |
| 2670 | C1CCc2ccccc2C1 | CCCCC=C | 0.22 | 0.31 | 0.08 | 0.34 | | 0.59 | 0.97 | | 0.40 | [118] |
| 2671 | C1CCc2ccccc2C1 | C1CCC=CC1 | 0.09 | 0.08 | 0.05 | 0.07 | | -0.11 | -0.16 | | 0.11 | [118] |
| 2672 | C1CCc2ccccc2C1 | C1CC=CC=C1 | 0.00 | -0.11 | 0.03 | 0.09 | | | | | -0.02 | [118] |
| 2673 | C1CCc2ccccc2C1 | C1C=CCC=C1 | -0.01 | -0.11 | 0.03 | 0.09 | | | | | -0.09 | [118] |
| 2674 | C1CCc2ccccc2C1 | CCCCCC=C | 0.25 | 0.35 | 0.10 | 0.36 | | 0.54 | 0.75 | | 0.42 | [118] |
| 2675 | C1CCc2ccccc2C1 | CCCCC#C | 0.09 | 0.62 | 0.34 | -0.29 | | | | | 0.19 | [118] |
| 2676 | C1CCc2ccccc2C1 | CCCCCC#C | 0.10 | 0.56 | 0.26 | -0.31 | | | | | 0.22 | [118] |
| 2677 | CN(C)CCN(C)C | CCCCCCC | 0.32 | 0.27 | 0.27 | 0.10 | | | | | 1.20 | [146] |
| 2678 | CN(C)CN(C)C | CCCCCCC | 0.16 | 0.33 | 0.33 | 0.09 | | | | | 1.30 | [146] |
| 2679 | CC(CN(C)C)N(C)C | CCCCCCC | | 0.22 | 0.22 | 0.10 | | | | | 1.20 | [146] |
| 2680 | OCCSCCO | CCCCCC | 3.48 | 2.70 | 2.63 | 3.95 | | 3.75 | 6.73 | | 4.50 | [84] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2681 | OCCSCCO | C1CCCCC1 | 2.95 | 2.39 | 2.19 | 3.71 | | 2.84 | 4.80 | | 4.02 | [84] |
| 2682 | OCCSCCO | CC1CCCC1 | 2.99 | 2.39 | 2.19 | 3.23 | | | | | 4.03 | [84] |
| 2683 | OCCSCCO | CCCCCCC | 3.92 | 3.12 | 3.00 | 4.36 | | 4.19 | 6.33 | | 4.91 | [84] |
| 2684 | OCCSCCO | CC1CCCCC1 | 3.34 | 2.83 | 2.57 | 3.88 | | 3.23 | 5.57 | | 4.40 | [84] |
| 2685 | OCCSCCO | CC(C)CC(C)(C)C | 3.93 | 3.53 | 3.42 | 4.75 | | 5.00 | 7.66 | | 4.84 | [84] |
| 2686 | OCCSCCO | c1ccccc1 | 1.31 | 1.28 | 1.03 | 1.57 | | 1.91 | 3.32 | | 2.17 | [84] |
| 2687 | OCCSCCO | Cc1ccccc1 | 1.75 | 1.58 | 1.23 | 1.82 | | 2.22 | 3.63 | | 2.73 | [84] |
| 2688 | N#CCCSCCC#N | C1CCCC1 | 3.29 | 1.86 | 1.90 | 3.32 | | | | | 3.37 | [200] |
| 2689 | N#CCCSCCC#N | CCCCCC | 4.52 | 2.77 | 2.77 | 4.37 | | | | | 4.65 | [200] |
| 2690 | N#CCCSCCC#N | C1CCCCC1 | 3.81 | 2.31 | 2.32 | 4.02 | | | | | 3.80 | [200] |
| 2691 | N#CCCSCCC#N | CCCC(C)C | 4.36 | 2.77 | 2.77 | 4.37 | | | | | 4.63 | [200] |
| 2692 | N#CCCSCCC#N | CCC(C)CC | 4.30 | 2.77 | 2.77 | 4.37 | | | | | 4.51 | [200] |
| 2693 | N#CCCSCCC#N | CC1CCCC1 | 3.87 | 2.30 | 2.31 | 3.50 | | | | | 3.89 | [200] |
| 2694 | N#CCCSCCC#N | CC(C)C(C)C | 4.15 | 2.77 | 2.76 | 4.37 | | | | | 4.45 | [200] |
| 2695 | N#CCCSCCC#N | CCCCCCC | 5.09 | 3.17 | 3.17 | 4.80 | | | | | 5.05 | [200] |
| 2696 | N#CCCSCCC#N | CC(C)CC(C)(C)C | 5.14 | 3.62 | 3.60 | 5.21 | | | | | 5.25 | [200] |
| 2697 | N#CCCSCCC#N | c1ccccc1 | 1.53 | 0.49 | 0.50 | 1.15 | | | | | 1.22 | [200] |
| 2698 | N#CCCSCCC#N | CCCCC=C | 3.45 | 0.18 | 0.19 | 3.52 | | | | | 3.78 | [200] |
| 2699 | N#CCCSCCC#N | C1CCC=CC1 | 2.84 | 0.35 | 0.36 | 2.78 | | | | | 2.88 | [200] |
| 2700 | N#CCCSCCC#N | CCOC(=O)C | 0.58 | 0.05 | 0.04 | 1.32 | | | | | 1.28 | [200] |
| 2701 | N#CCCSCCC#N | CCOCC | 1.93 | 1.02 | 1.03 | 2.48 | | | | | 2.17 | [200] |
| 2702 | N#CCCSCCC#N | CC(C)=O | -0.01 | -0.39 | -0.31 | 0.61 | | | | | 0.39 | [200] |
| 2703 | Cc1ccccc1 | CCCCC | 0.53 | 0.43 | 0.28 | 0.58 | 0.55 | 0.21 | 0.40 | 0.67 | 0.51 | [54 , 61 , 61 , 61 , 186] |
| 2704 | Cc1ccccc1 | CCCCCC | 0.58 | 0.46 | 0.32 | 0.54 | 0.58 | 0.21 | 0.31 | 0.65 | 0.57 | [54 , 61 , 61 , 61 , 78] |
| 2705 | Cc1ccccc1 | C1CCCCC1 | 0.44 | 0.30 | 0.28 | 0.45 | 0.32 | -0.12 | -0.11 | 0.41 | 0.44 | [54 , 61 , 61 , 65 , 78] |
| 2706 | Cc1ccccc1 | CCCC(C)C | 0.57 | 0.46 | 0.32 | 0.54 | 0.64 | | | 0.75 | 0.58 | [54 , 61 , 61] |
| 2707 | Cc1ccccc1 | CC1CCCC1 | 0.46 | 0.30 | 0.28 | 0.39 | 0.25 | | | 0.44 | 0.43 | [78] |
| 2708 | Cc1ccccc1 | CCCCCCC | 0.62 | 0.47 | 0.36 | 0.50 | 0.62 | 0.19 | 0.22 | 0.64 | 0.52 | [54 , 61 , 61 , 78] |
| 2709 | Cc1ccccc1 | CC(C)CC(C)C | 0.59 | 0.47 | 0.35 | 0.50 | 0.69 | | | 0.85 | 0.63 | [54 , 61 , 61] |
| 2710 | Cc1ccccc1 | CC1CCCCC1 | 0.49 | 0.33 | 0.31 | 0.43 | 0.26 | -0.01 | 0.04 | 0.49 | 0.35 | [78] |
| 2711 | Cc1ccccc1 | CCCCCCCC | 0.66 | 0.47 | 0.38 | 0.46 | 0.69 | 0.20 | 0.20 | 0.64 | 0.55 | [54 , 61 , 61 , 61] |
| 2712 | Cc1ccccc1 | C1CCCCCCC1 | 0.44 | 0.34 | 0.34 | 0.51 | 0.07 | -0.09 | -0.13 | 0.54 | 0.44 | [65] |
| 2713 | Cc1ccccc1 | CC(C)C(C)C(C)C | 0.57 | 0.46 | 0.38 | 0.46 | 0.43 | | | | 0.59 | [54 , 61 , 61] |
| 2714 | Cc1ccccc1 | CC(C)CCC(C)C | 0.64 | 0.46 | 0.38 | 0.46 | | | | | 0.65 | [54] |
| 2715 | Cc1ccccc1 | CCC1CCCCC1 | 0.52 | 0.34 | 0.34 | 0.40 | | | | 0.52 | 0.50 | [54 , 61] |
| 2716 | Cc1ccccc1 | CCCCCCCCC | 0.69 | 0.45 | 0.40 | 0.43 | 0.85 | 0.20 | 0.17 | 0.63 | 0.58 | [54 , 61 , 61] |
| 2717 | Cc1ccccc1 | CCC(C)CCC(C)C | 0.65 | 0.45 | 0.40 | 0.43 | | | | | 0.59 | [61] |
| 2718 | Cc1ccccc1 | c1ccccc1 | -0.04 | -0.04 | -0.03 | 0.01 | -0.05 | -0.22 | -0.24 | -0.04 | -0.01 | [61] |
| 2719 | Cc1ccccc1 | CCCC=C | 0.25 | 0.20 | 0.08 | 0.39 | 0.46 | 0.28 | 0.40 | 0.47 | 0.36 | [61] |
| 2720 | Cc1ccccc1 | CC(C)C=C | 0.26 | 0.20 | 0.08 | 0.39 | | | | | 0.31 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2721 | Cc1ccccc1 | CC(=C)C=C | 0.06 | 0.11 | 0.01 | 0.22 | 0.27 | | | | 0.17 | [61] |
| 2722 | Cc1ccccc1 | CCCCC=C | 0.29 | 0.23 | 0.10 | 0.37 | 0.46 | 0.21 | 0.35 | 0.46 | 0.29 | [61] |
| 2723 | Cc1ccccc1 | CO | 3.41 | 2.61 | 2.55 | 2.97 | 3.31 | 0.82 | 5.05 | 4.05 | 3.03 | [61 , 61] |
| 2724 | Cc1ccccc1 | CCO | 3.20 | 2.29 | 1.86 | 2.89 | 2.95 | 0.94 | 2.60 | 3.39 | 2.77 | [61 , 61] |
| 2725 | Cc1ccccc1 | CCOC(=O)C | 0.13 | -0.11 | -0.31 | 0.31 | 0.43 | 0.16 | -0.26 | 0.51 | 0.24 | [61] |
| 2726 | Cc1ccccc1 | C1COCCO1 | 0.23 | 1.08 | 0.39 | -0.15 | -0.19 | -0.08 | -0.03 | 0.06 | 0.14 | [61] |
| 2727 | Cc1ccccc1 | CCOCC | 0.10 | 0.13 | -0.05 | 0.22 | 0.25 | 0.18 | 0.08 | 0.18 | 0.01 | [61] |
| 2728 | Cc1ccccc1 | CC(C)=O | 0.49 | 0.38 | 0.24 | 0.56 | 0.79 | 0.28 | -0.17 | 0.53 | 0.70 | [61 , 61] |
| 2729 | Cc1ccccc1 | CCC(C)=O | 0.28 | 0.24 | 0.09 | 0.39 | 0.39 | 0.22 | -0.21 | 0.21 | 0.31 | [61] |
| 2730 | Cc1ccccc1 | c1ccncc1 | 0.33 | 0.32 | 0.31 | 0.38 | 0.13 | 0.09 | 0.28 | 0.52 | 2.99 | [201] |
| 2731 | Cc1ccccc1 | CCCCl | 0.01 | -0.09 | -0.20 | 0.03 | 0.07 | | | | 0.05 | [61] |
| 2732 | Cc1ccccc1 | CC(C)(C)Cl | 0.07 | 0.15 | -0.03 | 0.17 | 0.22 | | | | 0.17 | [61] |
| 2733 | Cc1ccccc1 | ClCCl | 0.03 | -0.24 | -0.27 | -0.14 | -0.11 | -0.20 | -0.17 | -0.13 | -0.14 | [61 , 61] |
| 2734 | Cc1ccccc1 | ClC(Cl)Cl | 0.05 | -0.49 | -0.53 | -0.30 | -0.22 | -0.20 | | -0.40 | -0.40 | [61] |
| 2735 | Cc1ccccc1 | ClC(Cl)(Cl)Cl | 0.49 | 0.00 | -0.11 | 0.00 | -0.04 | -0.20 | -0.21 | -0.01 | 0.02 | [61] |
| 2736 | Cc1ccccc1 | CCBr | -0.27 | 0.36 | 0.29 | 0.02 | 0.04 | -0.04 | | | -0.02 | [61] |
| 2737 | Cc1ccccc1 | CCC#N | 0.84 | 0.63 | 0.54 | 0.64 | 1.11 | 0.55 | 0.20 | 0.92 | 0.96 | [61] |
| 2738 | Cc1ccccc1 | CCI | -0.34 | 0.05 | 0.01 | 0.08 | 0.38 | | | | 0.06 | [61] |
| 2739 | Cc1ccccc1 | CCN(CC)CC | 0.28 | 0.06 | -0.06 | 0.15 | 0.19 | -0.12 | -0.13 | 0.26 | 0.19 | [61] |
| 2740 | Cc1ccccc1 | C(=S)=S | 0.00 | 0.15 | 0.22 | 0.23 | | -0.27 | -0.14 | | 0.23 | [61] |
| 2741 | CCCCOP(=O)(OCCCC)OCCCC | CCCCCC | 0.54 | | | | 0.70 | 0.07 | 0.60 | 0.73 | 0.63 | [202] |
| 2742 | CCCCOP(=O)(OCCCC)OCCCC | C1CCCCC1 | 0.39 | | | | 0.39 | -0.16 | -0.39 | 0.59 | 0.35 | [202] |
| 2743 | CCCCOP(=O)(OCCCC)OCCCC | CCCCCCC | 0.64 | | | | 0.92 | 0.15 | 0.40 | 0.91 | 0.66 | [202] |
| 2744 | CCCCOP(=O)(OCCCC)OCCCC | CCCCCCCC | 0.75 | | | | 1.20 | 0.24 | 0.33 | 1.08 | 0.96 | [202] |
| 2745 | CCCCOP(=O)(OCCCC)OCCCC | c1ccccc1 | -0.31 | | | | -0.45 | -0.31 | -0.62 | -0.60 | -0.45 | [202] |
| 2746 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CO | 1.10 | | | | | -0.36 | 4.15 | | 0.65 | [203] |
| 2747 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCO | 1.30 | | | | | -0.04 | 0.50 | | 0.68 | [203] |
| 2748 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCCO | 1.21 | | | | | 0.21 | -0.54 | | 0.65 | [203] |
| 2749 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCCCO | 1.19 | | | | | 0.43 | -0.71 | | 0.78 | [203] |
| 2750 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CC(=O)OC | -0.04 | | | | | -0.40 | 1.64 | | -0.09 | [203] |
| 2751 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCOC(=O)C | -0.13 | | | | | -0.40 | 1.64 | | -0.05 | [203] |
| 2752 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCCOC(=O)C | -0.14 | | | | | 0.31 | 3.21 | | 0.03 | [203] |
| 2753 | CC1=CC=C(C=C1)OP(=O)(OC2=CC=C(C=C2)C)OC3=CC=C(C=C3)C | CCCCOC(=O)C | -0.13 | | | | | 0.43 | 3.58 | | 0.16 | [203] |
| 2754 | CCN(CC)CC | CCCCC | 0.07 | 0.01 | 0.02 | 0.04 | | 0.07 | 0.38 | 0.01 | 0.00 | [54 , 61 , 61] |
| 2755 | CCN(CC)CC | CCCCCC | 0.10 | 0.04 | 0.04 | 0.04 | | 0.07 | 0.27 | 0.05 | 0.03 | [54 , 61 , 61] |
| 2756 | CCN(CC)CC | C1CCCCC1 | 0.09 | 0.04 | 0.03 | 0.20 | | -0.24 | -0.21 | 0.22 | 0.12 | [54 , 61 , 61] |
| 2757 | CCN(CC)CC | CCCC(C)C | 0.09 | 0.04 | 0.04 | 0.04 | | | | 0.04 | 0.04 | [54 , 61 , 61] |
| 2758 | CCN(CC)CC | CCCCCCC | 0.11 | 0.05 | 0.05 | 0.05 | | 0.05 | 0.18 | 0.10 | 0.08 | [54] |
| 2759 | CCN(CC)CC | CC(C)CC(C)C | 0.10 | 0.05 | 0.05 | 0.05 | | | | 0.08 | 0.04 | [54 , 61 , 61] |
| 2760 | CCN(CC)CC | CCCCCCCC | 0.13 | 0.04 | 0.05 | 0.05 | | 0.06 | 0.15 | 0.13 | 0.04 | [54 , 61] |
| 2761 | CCN(CC)CC | CC(C)C(C)C(C)C | 0.10 | 0.04 | 0.05 | 0.05 | | | | | 0.09 | [54 , 61] |
| 2762 | CCN(CC)CC | CC(C)CCC(C)C | 0.12 | 0.04 | 0.05 | 0.05 | | | | | 0.13 | [54] |
| 2763 | CCN(CC)CC | CCC1CCCCC1 | 0.13 | 0.09 | 0.05 | 0.21 | | | | 0.26 | 0.09 | [54 , 61] |
| 2764 | CCN(CC)CC | CCCCCCCCC | 0.14 | 0.03 | 0.05 | 0.05 | | 0.07 | 0.11 | 0.16 | 0.13 | [54 , 61] |
| 2765 | CCN(CC)CC | Cc1ccccc1 | 0.24 | 0.05 | -0.04 | 0.20 | | -0.26 | -0.26 | 0.13 | 0.19 | [61] |

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**Table S6 – continued from previous page**

| ID | Solvent SMILES | Solute SMILES | COSMO-RS | UNIFAC | UNIFAC (Ly) | UNIFAC (Do) | Abraham | HSP | Hildebrand | MOSCED | Literature | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2766 | CCN(CC)CC | CCO | 0.81 | 0.71 | 0.63 | 1.53 | | 0.99 | 3.72 | 1.68 | 0.67 | [61] |
| 2767 | CCN(CC)CC | C1COCCO1 | 0.65 | 1.35 | 1.12 | 0.52 | | -0.09 | 0.04 | 1.11 | 0.92 | [61] |
| 2768 | CCN(CC)CC | CCC(C)=O | 0.72 | 0.97 | 1.01 | 0.96 | | 0.23 | -0.25 | 0.97 | 1.07 | [61] |
| 2769 | C(COCCOCCO)O | CCCCCC | 2.70 | 2.43 | 2.39 | 3.13 | | 3.81 | 2.49 | | 4.14 | [144 , 47 , 73] |
| 2770 | C(COCCOCCO)O | C1CCCCC1 | 2.28 | 2.14 | 1.98 | 2.95 | | 2.99 | 1.17 | | 3.43 | [144] |
| 2771 | C(COCCOCCO)O | CCCCCCC | 3.06 | 2.84 | 2.74 | 3.49 | | 4.30 | 2.22 | | 4.59 | [144] |
| 2772 | C(COCCOCCO)O | CC1CCCCC1 | 2.59 | 2.56 | 2.34 | 3.10 | | 3.38 | 1.69 | | 3.85 | [144] |
| 2773 | C(COCCOCCO)O | CCCCCCCC | 3.42 | 3.22 | 3.09 | 3.84 | | 4.79 | 2.10 | | 4.96 | [144] |
| 2774 | C(COCCOCCO)O | CC(C)CC(C)(C)C | 3.05 | 3.23 | 3.13 | 3.84 | | 5.01 | 3.20 | | 4.76 | [144] |
| 2775 | C(COCCOCCO)O | CCC1CCCCC1 | 2.93 | 2.97 | 2.70 | 3.47 | | | | | 4.21 | [144] |
| 2776 | C(COCCOCCO)O | CCCCCCCCC | 3.78 | 3.60 | 3.43 | 4.20 | | 5.30 | 1.98 | | 5.34 | [144] |
| 2777 | C(COCCOCCO)O | c1ccccc1 | 0.98 | 1.00 | 0.80 | 1.42 | | 2.12 | 0.31 | | 1.48 | [144 , 47 , 73] |
| 2778 | C(COCCOCCO)O | Cc1ccccc1 | 1.35 | 1.42 | 1.12 | 1.64 | | 2.40 | 0.51 | | 1.79 | [144] |
| 2779 | C(COCCOCCO)O | Cc1cccc(C)c1 | 1.65 | 1.78 | 1.39 | 1.86 | | 2.66 | 0.58 | | 2.29 | [144] |
| 2780 | C(COCCOCCO)O | Cc1ccc(C)cc1 | 1.67 | 1.78 | 1.39 | 1.86 | | 2.62 | 0.66 | | 2.29 | [144] |
| 2781 | C(COCCOCCO)O | Cc1ccccc1C | 1.57 | 1.78 | 1.39 | 1.86 | | 2.59 | 0.57 | | 2.16 | [144] |
| 2782 | C(COCCOCCO)O | CCc1ccccc1 | 1.64 | 1.84 | 1.48 | 2.26 | | 3.12 | 0.67 | | 2.23 | [144] |
| 2783 | C(COCCOCCO)O | CCCc1ccccc1 | 1.97 | 2.21 | 1.80 | 2.63 | | | | | 2.67 | [144] |
| 2784 | C(COCCOCCO)O | CC(C)c1ccccc1 | 1.88 | 2.25 | 1.83 | 2.50 | | 3.62 | 0.58 | | 2.62 | [144] |
| 2785 | C(COCCOCCO)O | CCC\C=C/C | 2.04 | 2.28 | 2.24 | 2.68 | | | | | 3.43 | [144] |
| 2786 | C(COCCOCCO)O | C1CCC=CC1 | 1.72 | 2.00 | 1.84 | 2.20 | | 1.70 | 0.58 | | 2.75 | [144] |
| 2787 | C(COCCOCCO)O | CCCCCC=C | 2.40 | 2.70 | 2.61 | 3.03 | | 3.14 | 2.24 | | 3.90 | [144] |
| 2788 | C(COCCOCCO)O | CCCCCCC=C | 2.80 | 3.09 | 2.95 | 3.40 | | 3.46 | 2.07 | | 4.31 | [144] |
| 2789 | C(COCCOCCO)O | CC(=C)CC(C)(C)C | 2.49 | 3.11 | 3.06 | 3.42 | | | | | 4.17 | [144] |
| 2790 | OC(F)(F)CF | CCCCC | 3.06 | 2.44 | 2.24 | 3.50 | 3.23 | 2.28 | 2.50 | | 3.17 | [54] |
| 2791 | OC(F)(F)CF | CCCCCC | 3.53 | 2.82 | 2.58 | 3.86 | 3.69 | 2.60 | 2.30 | | 3.75 | [54] |
| 2792 | OC(F)(F)CF | C1CCCCC1 | 3.17 | 2.64 | 2.18 | 3.63 | 3.78 | 2.11 | 1.38 | | 3.67 | [54] |
| 2793 | OC(F)(F)CF | CCCC(C)C | 3.40 | 2.82 | 2.58 | 3.86 | 3.60 | | | | 3.56 | [54] |
| 2794 | OC(F)(F)CF | CCCCCCC | 3.98 | 3.18 | 2.92 | 4.22 | 4.15 | 2.93 | 2.11 | | 4.23 | [54] |
| 2795 | OC(F)(F)CF | CC(C)CC(C)C | 3.69 | 3.18 | 2.91 | 4.22 | 3.92 | | | | 3.85 | [54] |
| 2796 | OC(F)(F)CF | CCCCCCCC | 4.43 | 3.53 | 3.24 | 4.57 | 4.65 | 3.26 | 2.02 | | 4.73 | [54] |
| 2797 | OC(F)(F)CF | CC(C)C(C)C(C)C | 3.94 | 3.53 | 3.24 | 4.57 | 4.22 | | | | 4.20 | [54] |
| 2798 | OC(F)(F)CF | CC(C)CCC(C)C | 4.17 | 3.53 | 3.24 | 4.57 | | | | | 4.33 | [54] |
| 2799 | OC(F)(F)CF | CCC1CCCCC1 | 3.96 | 3.39 | 2.85 | 4.15 | | | | | 4.47 | [54] |
| 2800 | OC(F)(F)CF | CCCCCCCCC | 4.88 | 3.86 | 3.57 | 4.93 | 5.23 | 3.60 | 1.93 | | 5.20 | [54] |
| 2801 | O=[S]1(=O)CCC(C1)C=C | C1CCCC1 | | 1.58 | 1.62 | 2.69 | | | | | 2.53 | [84] |
| 2802 | O=[S]1(=O)CCC(C1)C=C | CCCCCC | | 2.42 | 2.36 | 3.59 | | | | | 3.52 | [84] |
| 2803 | O=[S]1(=O)CCC(C1)C=C | C1CCCCC1 | | 1.96 | 1.98 | 3.26 | | | | | 2.94 | [84] |
| 2804 | O=[S]1(=O)CCC(C1)C=C | CC1CCCC1 | | 1.96 | 1.97 | 2.87 | | | | | 2.98 | [84] |
| 2805 | O=[S]1(=O)CCC(C1)C=C | CCCCCCC | | 2.76 | 2.70 | 3.96 | | | | | 3.86 | [84] |
| 2806 | O=[S]1(=O)CCC(C1)C=C | CC1CCCCC1 | | 2.32 | 2.32 | 3.43 | | | | | 3.30 | [84] |
| 2807 | O=[S]1(=O)CCC(C1)C=C | CC(C)CC(C)(C)C | | 3.15 | 3.07 | 4.33 | | | | | 3.97 | [84] |
| 2808 | O=[S]1(=O)CCC(C1)C=C | c1ccccc1 | | 0.32 | 0.36 | 0.67 | | | | | 0.83 | [84] |
| 2809 | O=[S]1(=O)CCC(C1)C=C | Cc1ccccc1 | | 0.58 | 0.58 | 0.92 | | | | | 1.16 | [84] |

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