Density of deep eutectic solvents: The path forward cheminformatics-driven reliable predictions for mixtures

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Table S5. Models CO54, MO75 and CO17 derived for the DES' density (ρ in g/cm^3) along with their statistical parameters.

Model	Equation	Training set results	Test set results
CO54	$\rho = +1.180(\pm0.020) - 0.083(\pm0.003)\mathrm{TI2\_L_{pmix}} + 0.348(\pm0.022)\mathrm{SM1\_Dz(Z)_{pmix}} + 0.027(\pm0.001)\mathrm{Eta\_F_{pmix}} - 0.028(\pm0.001)\mathrm{ALOGP_{pmix}} - 0.112(\pm0.006)\mathrm{rGes_{nmix}} + 0.059(\pm0.006)\mathrm{SpMin2\_Bh(s)_{pmix}} - 0.0004(\pm0.0000)T(\mathrm{K})$	$N_{training}$ = 854; R^2 = 0.883; R^2_{Adj} = 0.882; $F(7,846)$ = 914.3; Q^2_{LOO} = 0.881; MAE_{LOO} = 0.025; $r_m^2{}_{(LOO)}$ = 0.831; $\Delta r_m^2{}_{(LOO)}$ = 0.099; Q^2_{LCO} =0.838; MAE_{LCO} = 0.030; $\%AARD_{tr}$ = 2.186	N_{test} = 300; R^2_{Pred} = 0.803; MAE_{test} =0.030, $r_m^2{}_{(test)}$ = 0.662; $\Delta r_m^2{}_{(test)}$ = 0.114; $\%AARD_{test}$ = 2.491
MO75	$\rho = +1.120(\pm0.021) - 0.020(\pm0.003)\mathrm{S3K_{pmix}} + 0.346(\pm0.012)\mathrm{SM1\_Dz(m)_{pmix}} + 0.028(\pm0.002)\mathrm{SpMax\_EA(dm)_{pmix}} + 0.013(\pm0.000)\mathrm{MLOGP2_{pmix}} - 0.0004(\pm0.0000)T(\mathrm{K})$	$N_{training}$ = 856; R^2 = 0.867; R^2_{Adj} = 0.866; $F(5,850)$ = 914.3; Q^2_{LOO} =0.865; MAE_{LOO} = 0.025; $r_m^2{}_{(LOO)}$ = 0.807; $\Delta r_m^2{}_{(LOO)}$ = 0.113; Q^2_{LCO} =0.844; MAE_{LCO} = 0.027; $\%AARD_{tr}$ = 2.246	N_{test} = 298; R^2_{Pred} = 0.802; MAE_{test} =0.028, $r_m^2{}_{(test)}$ = 0.726; $\Delta r_m^2{}_{(test)}$ = 0.101; $\%AARD_{test}$ = 1.750
CO17	$\rho = +0.913(\pm0.013) + 0.044(\pm0.001)\mathrm{AMW_{pmix}} - 0.055(\pm0.006)\mathrm{Psi\_i\_1d_{pmix}} + 0.032(\pm0.002)\mathrm{SpMax7\_Bh(e)_{pmix}} + 0.119(\pm0.010)\mathrm{nRNHR_{pmix}} + 0.010(\pm0.000)\mathrm{MLOGP2_{pmix}} + 0.013(\pm0.001)\mathrm{SM13\_AEA(dm)_{nmix}} - 0.011(\pm0.000)\mathrm{ATSC8m_{pmix}} + 0.741(\pm0.019)\mathrm{ATSC1e_{pmix}} - 0.032(\pm0.002)\mathrm{CATS2D\_02\_DL_{nmix}} - 0.001(\pm0.0000)T(\mathrm{K})$	$N_{training}$ = 837; R^2 = 0.930; R^2_{Adj} = 0.929; $F(10,826)$ = 1095; Q^2_{LOO} = 0.927; MAE_{LOO} = 0.014; $r_m^2{}_{(LOO)}$ = 0.895; $\Delta r_m^2{}_{(LOO)}$ = 0.062; Q^2_{LCO} = 0.891; MAE_{LCO} = 0.017; $\%AARD_{train}$ = 1.136	N_{test} = 317; R^2_{Pred} = 0.879; MAE_{test} =0.041; $r_m^2{}_{(test)}$ = 0.627; $\Delta r_m^2{}_{(test)}$ = 0.116; $\%AARD_{test}$ = 3.927