Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Gamma-Valerolactone + Toluene

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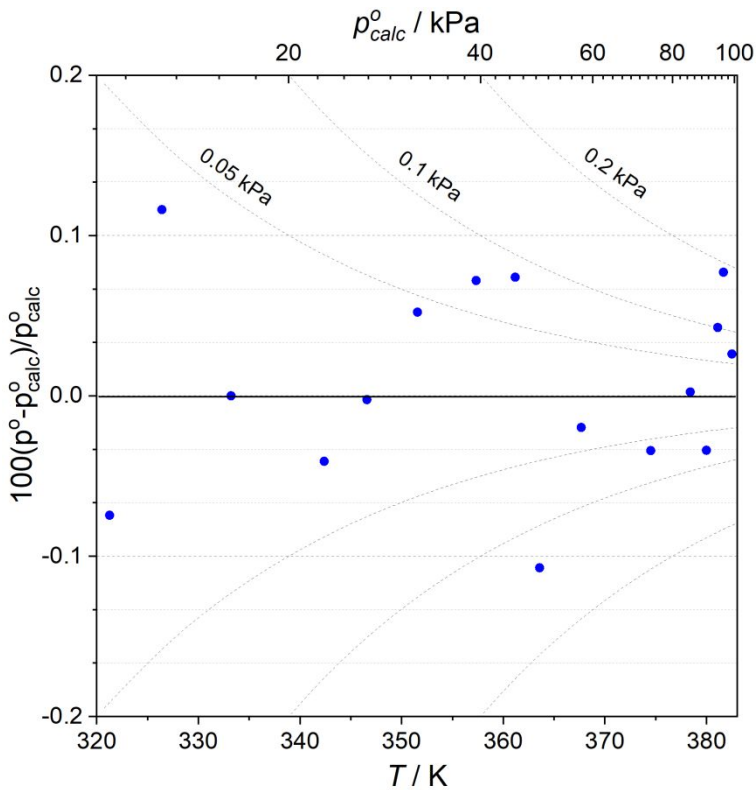

Figure S1 Deviation of experimental vapor pressures (p^o_{meas}) from the Antoine equation fit (p^o_{calc}) for toluene (●)

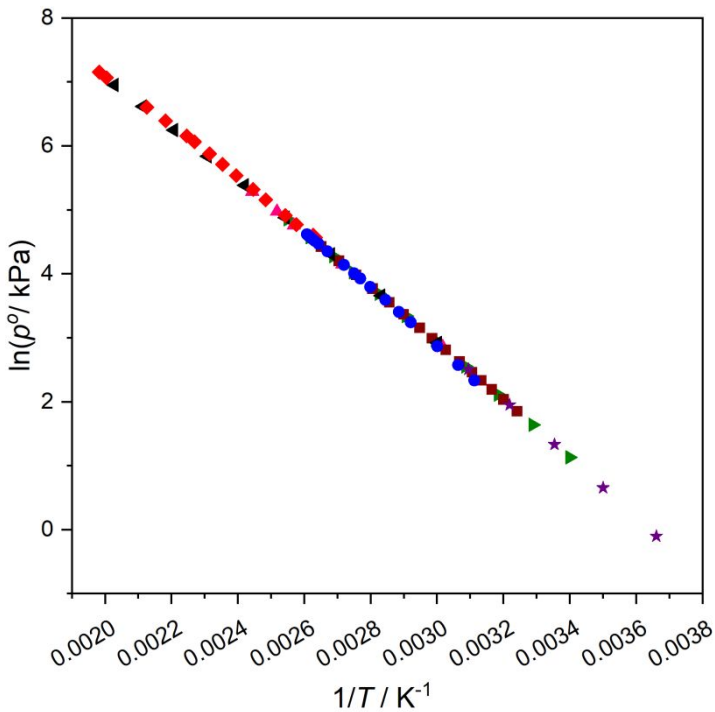

Figure S2 ln(p^o) – 1/T plot for toluene. blue ●: this work, red ◆: Wiswanath et al., black ◀□: Eubank et al, brown ■: Willingham et al, dark purple ★: Pitzer et al, pink ▲: Holder et al, green ▶: Jose et al

Table S1 Refractive indices of Toluene (1) – GVL (2) binary mixtures at T = 293.15 K, and p = 101.3 kPa. u(p) = 0.5 kPa, u(T) = 0.1 K

Mole fraction of Toluene (x_1 / –)	n_D^{20} / –	Mole fraction of Toluene (x_1 / –)	n_D^{20} / –
1.0000	1.4972	0.4297	1.4620
0.9737	1.4956	0.4071	1.4603
0.8632	1.4891	0.3517	1.4564
0.8273	1.4869	0.3047	1.4539
0.7801	1.4837	0.2463	1.4500
0.7110	1.4798	0.2008	1.4472
0.7047	1.4791	0.1299	1.4421
0.6166	1.4733	0.0000	1.4338
0.5094	1.4667		

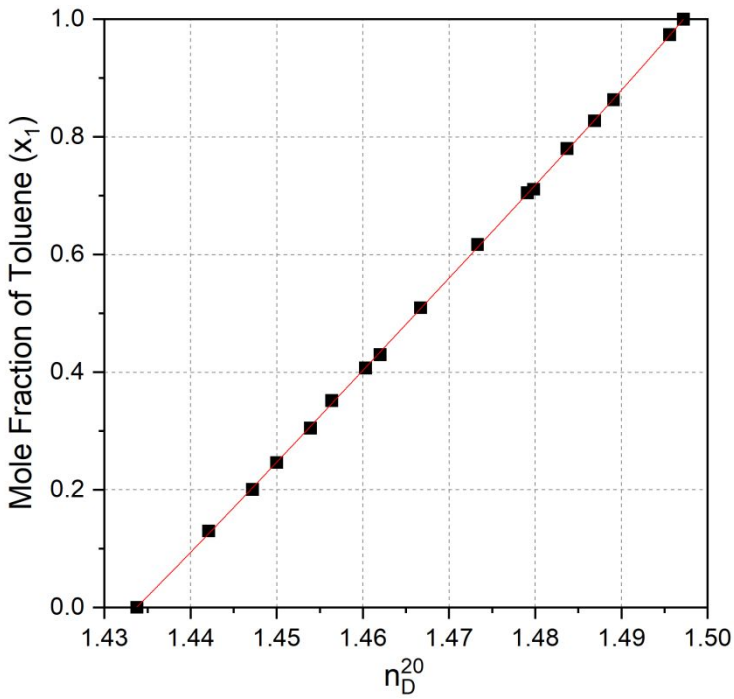

Figure S3 Experimental Refractive Indexes of the Toluene (1) – GVL (2) System at 293.15 K

Table S2 Structural Parameters for the UNIFAC and UNIQUAC models (R –Volume Parameter, Q – Area Parameter, r – van der Waals volume parameter, q – van der Waals area parameter) for Pure Components

Parameter	Toluene	GVL[a]
R	3.9228	3.6988
Q	2.968	3.036
r	3.9228	R_{GVL}
q	2.9679	Q_{GVL}

[a] GVL was divided in ChemCAD to the following subgroups for calculating R and Q parameters for the UNIFAC model: subgroups 1 (CH_3), 2 (CH_2), 3 (CH) and 23 (CH_2COO) were included. Toluene was divided to subgroups 10 (ACH – 5 units) and 12 ($ACHCH_2$).[1] As the r and q parameters for GVL are not available, ChemCAD applied r and q from UNIFAC model.

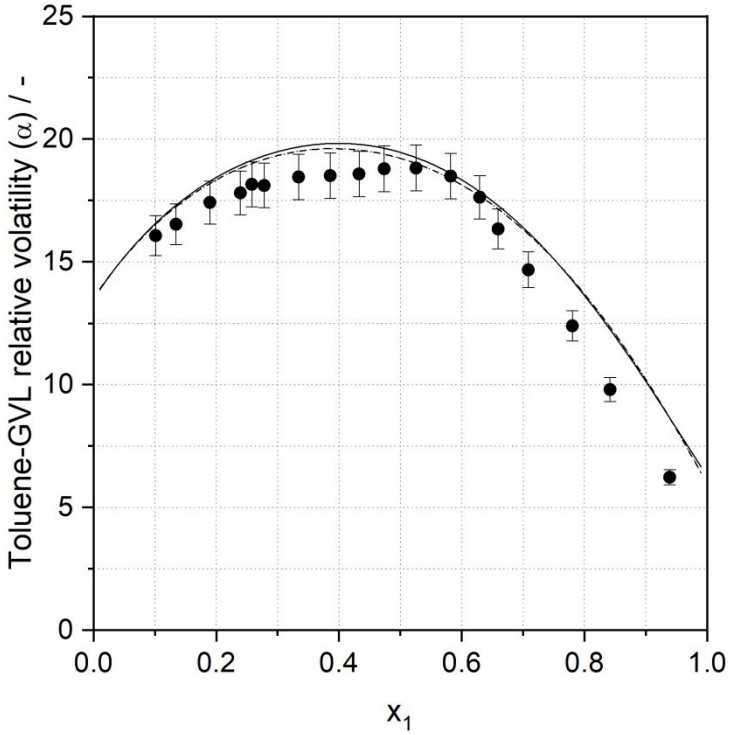

Figure S4 Relative volatility plot of the Toluene – GVL binary system at p = 101.3 kPa.
─ UNIQUAC model, --- NRTL model,····· Wilson model

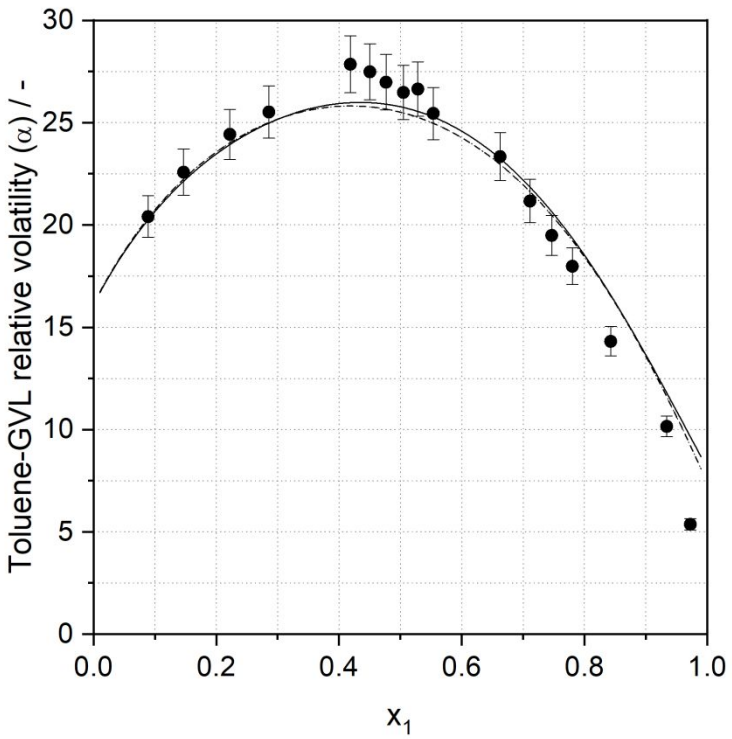

Figure S5 Relative volatility plot of the Toluene – GVL binary system at p = 50.7 kPa.
─ UNIQUAC model, --- NRTL model,····· Wilson model

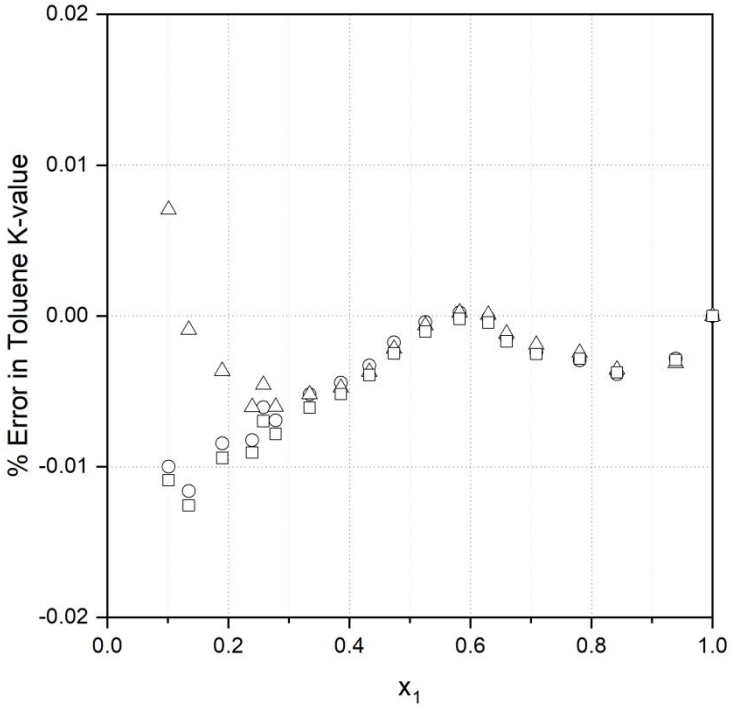

Figure S6 Percentage errors of model K_1-values of Toluene in VLE data of Toluene-GVL binary mixture at p = 101.3 kPa. □: UNIQUAC model, △: NRTL model ○: Wilson model

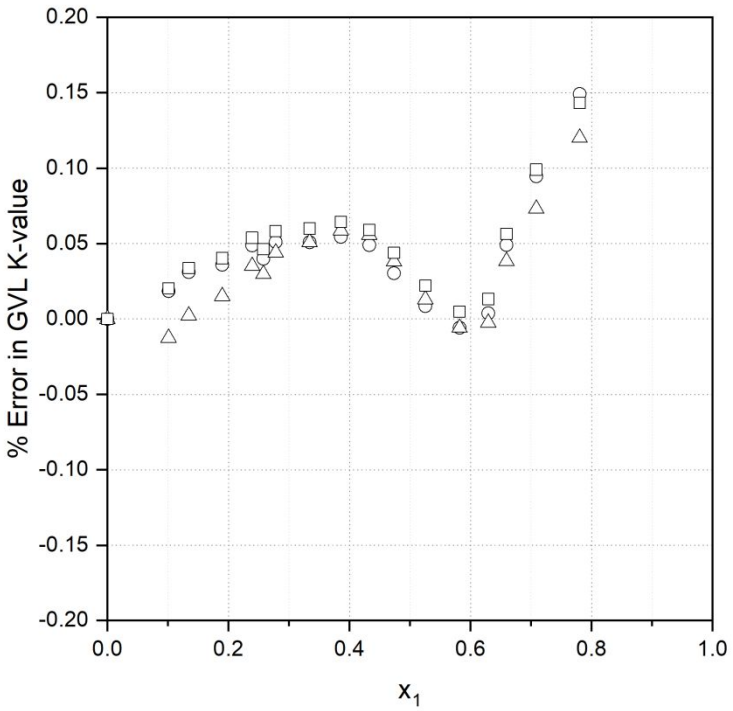

Figure S7 Percentage errors of model K_2-values of GVL in VLE data of Toluene-GVL binary mixture at p = 101.3 kPa. □: UNIQUAC model, △: NRTL model ○: Wilson model

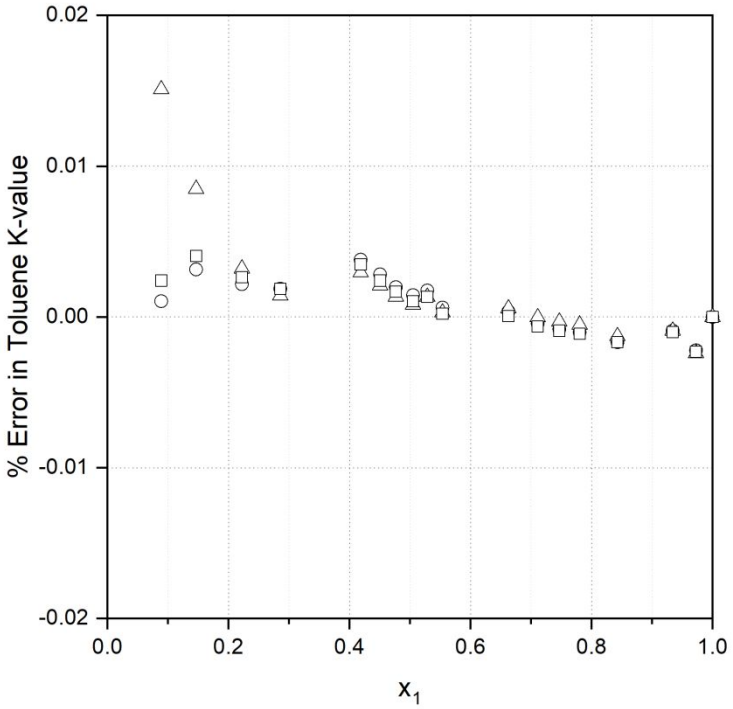

Figure S8 Percentage errors of model K_1-values of Toluene in VLE data of Toluene-GVL binary mixture at p = 50.05 kPa. □: UNIQUAC model, △: NRTL model ○: Wilson model

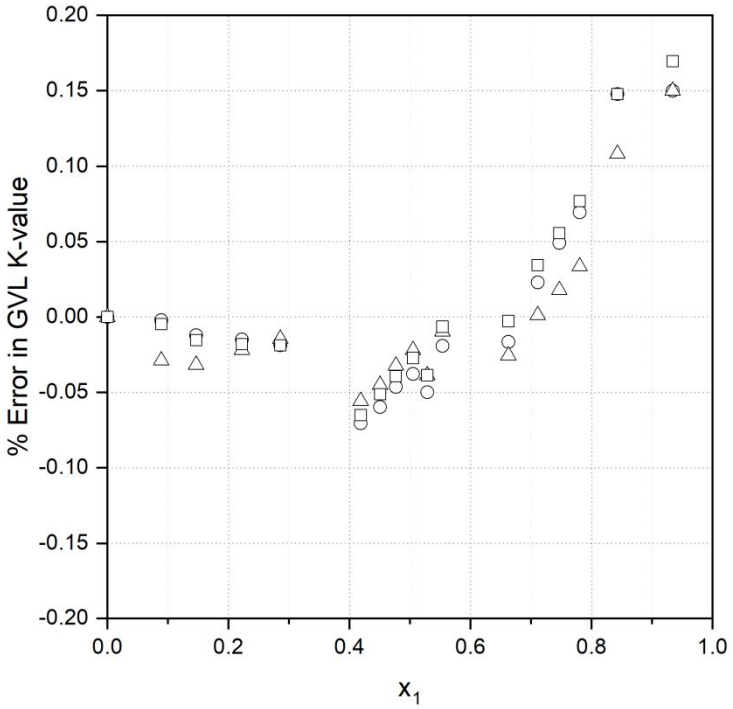

Figure S9 Percentage errors of model K_2-values of GVL in VLE data of Toluene-GVL binary mixture at p = 50.7 kPa. □: UNIQUAC model, △: NRTL model ○: Wilson model

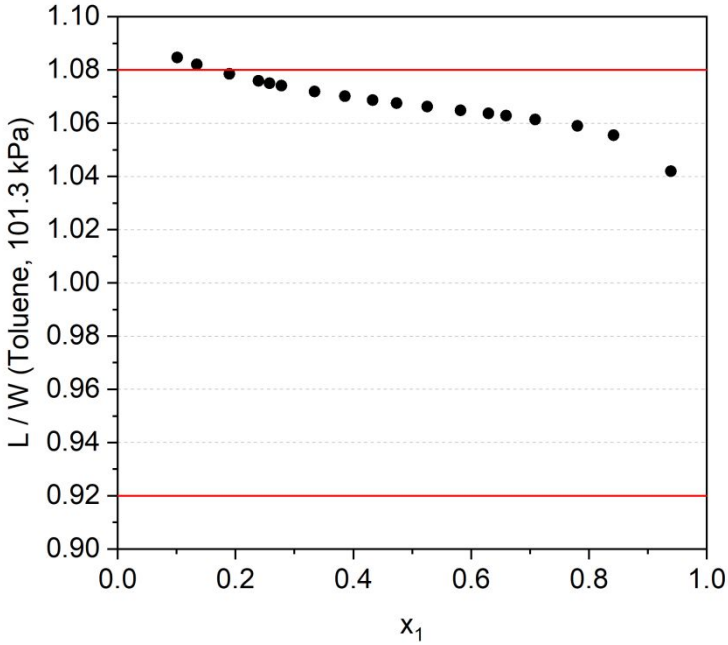

Figure S10 L/W coefficients of the Wisniak test for toluene – GVL system at 101.3 kPa.

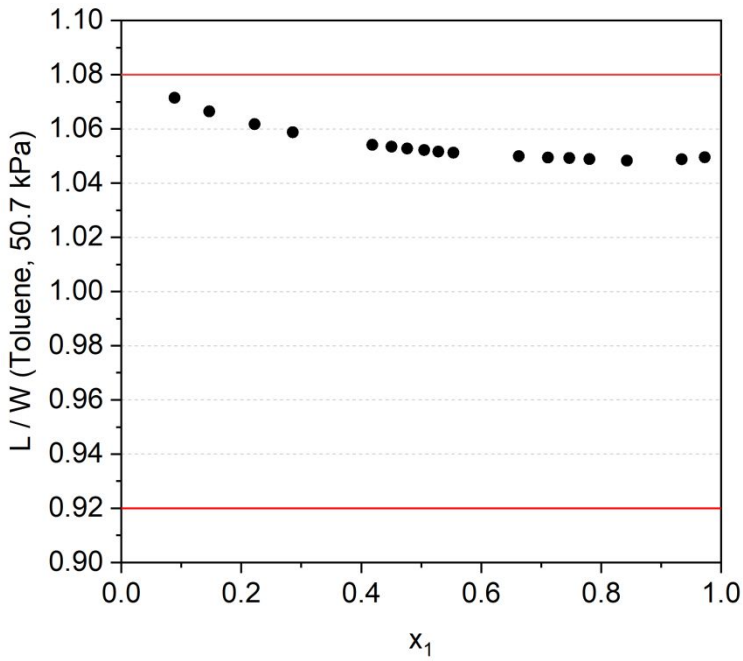

Figure S11 L/W coefficients of the Wisniak test for toluene – GVL system at 50.7 kPa.

References

(1) Gmehling, J.; Rasmussen, P.; Fredenslund, A. Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension. 2. *Ind. Chem. Process. Des. Dev*. **1982**, *21*, 118–127.