



Data Article

Dataset for the interfacial tension and phase properties of the ternary system water – 2-butoxyethanol – toluene



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ABSTRACT

Two-phase samples containing water, 2-butoxyethanol, and toluene in the different mass ratios were gravimetrically prepared in the jacketed cells at $T=293.15$ K and $p=0.100$ MPa and equilibrated for 24 h. The samples were volumetrically titrated until homogeneous. Then new samples were prepared in the two-phase region with compositions in the immediate proximity to the expected separation boundary and titrated until homogeneous. The critical point was located, keeping the phase ratio of 1:1 during the titration. The density of homogeneous samples obtained during titration was measured using the density meter. These data were used to construct an interpolation of the density along the separation boundary. New two-phase samples were prepared; the interfacial tension, density, and viscosity were measured. Thus, interfacial tension isotherm and viscosity isotherm were obtained using density interpolation to determine the composition of the equilibrated phases.

The obtained data can be used to prepare the two-phase samples with desired properties, design the oil-water

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separation processes, and develop new oil spill dispersants containing 2-butoxyethanol.

This article is a co-submission with a paper [1].

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Specifications Table

Subject	Chemistry
Specific subject area	Surface and colloid chemistry
Type of data	Tables, figures
How the data were acquired	The location of the phase separation boundary on the water – 2-butoxyethanol – toluene diagram was determined by volumetric titration. At first, two-phase samples containing water, 2-butoxyethanol (BEG), and toluene (TOL) in the different mass ratios were gravimetrically prepared using the balances PA413C (Ohaus, USA). The comparison with other ternary systems containing BEG (or MeEG) was conducted using available literature presented in references. The density of homogeneous samples obtained during titration was measured using the density meter DMA 4500 (Anton Paar, Austria). These data were used to construct an interpolation of the density along the separation boundary, which was applied to determine the compositions of equilibrated phases of heterogeneous samples. A spinning drop tensiometer SDT (Krüss, Hamburg, Germany) and a force tensiometer K20 (Krüss, Hamburg, Germany) were used to measure the interfacial tension in the two-phase region. The density and dynamic viscosity of equilibrated phases were measured with a rolling-ball viscometer Lovis 2000 ME (Anton Paar, Austria) integrated with a density meter DMA 4500.
Data format	Raw and analyzed
Parameters for data collection	The samples of the ternary system were prepared in the laboratory.
Description of data collection	Phase diagram, interfacial tension isotherm, density, and viscosity for the ternary system water – 2-butoxyethanol – toluene.
Data source location	Gubkin University, Department of Physical and Colloid Chemistry. Moscow, Russia
Data accessibility	With the article
Related research article	Alexandra A. Kuchierskaya, Anton P. Semenov, Adeliya R. Sayfutdinova, Dmitry S. Kopitsyn, Vladimir A. Vinokurov, Mikhail A. Anisimov, Andrei A. Novikov. Interfacial tension and phase properties of water – hydrotrope – oil solutions: water – 2-butoxyethanol – toluene. <i>Journal of Molecular Liquids</i> 344 (2021) 117683 [1].

Value of the data

- In this work, we compared behavior of hydrotropes – tertiary butanol (TBA) and 2-butoxyethanol (BEG) – at the oil/water interface. It shows a high degree of universality, however, more hydrophobic BEG demonstrates higher adsorption at the oil/water interface and shifts the critical point closer to the water vertex. These results could be used to predict the behavior of the systems with different hydrotropes.
- The present data on the phase equilibria can be useful in constructing phase diagrams of ternary systems containing low-molecular-weight amphiphiles.
- It has been shown that measuring density along the separation boundary can be used to determine the composition of equilibrium phases in the two-phase region with a high accuracy.
- Data on interfacial tension, density, and viscosity could be used to rationally design oil spill dispersants.

1. Data Description

The data on phase equilibrium and interfacial phenomena of the system water – BEG – toluene is reported in this work in accordance with recent IUPAC recommendations [2]. Compositions of two-phase and one-phase samples along the phase separation boundary are presented in Table 1. Data in Table 1 include the densities of water – BEG – toluene homogeneous systems obtained during titration, which were further used to construct an interpolation of the density along the separation boundary (Fig. 1). Approximated binodal curves at 293.15 K for ternary water – BEG – toluene and water – TBA – toluene systems and fitting residuals are shown in Fig. 2 (the data for the Fig. 2 construction are in Table 2). The ternary phase diagrams of water – BEG – toluene and water – TBA – toluene systems at 293.15 K are shown in Fig. 3. The comparison of water – BEG – toluene with other ternary systems containing BEG (or MeEG) is presented in Fig. 4. Compositions of water – BEG – toluene system samples used to construct

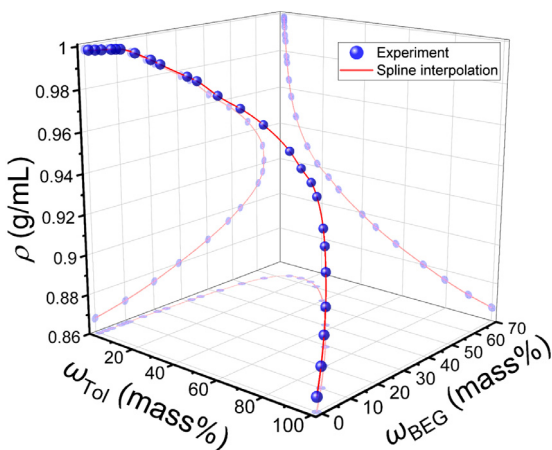


Fig. 1. Density at the separation boundary as a function of the composition for the ternary system of H₂O-BEG-TOL at 293.15 K; spheres – experimental data, red line – cubic spline interpolation, projections of experimental points and interpolation curve on the XY, XZ, YZ planes are shown. Data are from Table 1 (ω_{Tol} is from Column III; ω_{BEG} is from Column VI; ρ is from Column XIV).

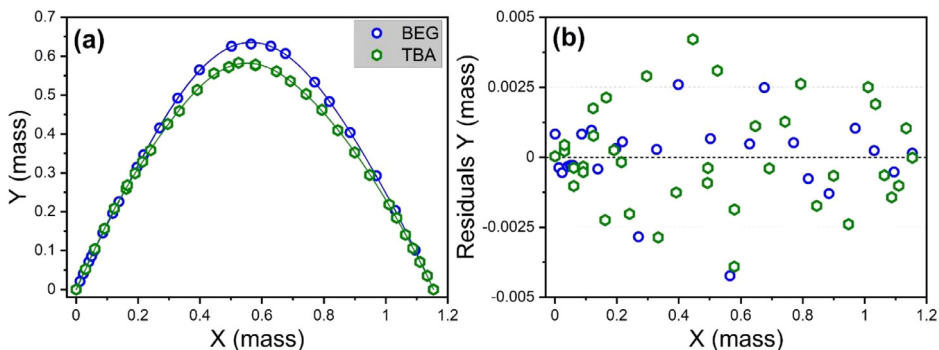


Fig. 2. (a) Binodal curves at 293.15 K for ternary systems of H₂O-TBA-TOL [6] and H₂O-BEG-TOL (this work) approximated by 9th order polynomial; (b) fitting residuals; (Y is mass fraction of hydrotrope ω_h , $X = (2 \times \omega_{\text{TOL}} + \omega_h)/\sqrt{3}$); (a) circles and hexagons are experimental data (titration); blue and green curves are polynomial approximations. Data are from Table 2 (X is from Column II, Y is from Column III, residuals Y are from Column IV).

Table 1Phase separation boundary and density data on H₂O–BEG–TOL system at $T=293.15$ K and $p=0.100$ MPa obtained by titration.^a

Point number I	Two-phase points Mass fraction			One-phase points Mass fraction			Two-phase points Mole fraction			One-phase points Mole fraction			ρ , g/mL (one-phase state) XIV
	H ₂ O II	BEG III	TOL IV	H ₂ O V	BEG VI	TOL VII	H ₂ O VIII	BEG IX	TOL X	H ₂ O XI	BEG XII	TOL XIII	
1	0.99909	0	0.00091	0.99910	0	0.00090	0.99982	0	0.00018	0.99982	0	0.00018	0.99821
2	0.9788	0.0206	0.0006	0.9787	0.0207	0.0006	0.99668	0.00320	0.00012	0.99666	0.00321	0.00013	0.99769
3	0.9595	0.0401	0.0004	0.9595	0.0402	0.0004	0.99359	0.00633	0.00008	0.99359	0.00634	0.00007	0.99729
4	0.9283	0.0713	0.0004	0.9285	0.0711	0.0004	0.98834	0.01157	0.00008	0.98839	0.01154	0.00007	0.99671
5	0.9139	0.0854	0.0006	0.9139	0.0855	0.0006	0.98583	0.01404	0.00013	0.98581	0.01406	0.00013	0.99644
6	0.89954	0.09943	0.00103	0.89958	0.09940	0.00102	0.98321	0.01657	0.00022	0.98322	0.01656	0.00022	0.99613
7	0.85249	0.14519	0.00232	0.85251	0.14518	0.00231	0.97419	0.02529	0.00052	0.97419	0.02529	0.00052	0.99311
8	0.7995	0.1955	0.0050	0.7996	0.1955	0.0049	0.96293	0.03589	0.00118	0.96295	0.03589	0.00116	0.98863
9	0.7673	0.2261	0.0066	0.7671	0.2254	0.0075	0.95547	0.04292	0.00161	0.95538	0.04279	0.00183	0.98567
10	0.6723	0.3144	0.0134	0.6726	0.3141	0.0133	0.93007	0.06630	0.00362	0.93018	0.06623	0.00359	0.97725
11	0.6362	0.3482	0.0156	0.6376	0.3465	0.0159	0.91893	0.07667	0.00441	0.91934	0.07617	0.00449	0.97414
12	0.5588	0.4151	0.0261	0.5587	0.4153	0.0260	0.89097	0.10089	0.00814	0.89095	0.10094	0.00810	0.96474
13	0.4696	0.4917	0.0387	0.4697	0.4918	0.0385	0.85054	0.13576	0.01370	0.85059	0.13578	0.01363	0.95584
14	0.3724	0.5647	0.0629	0.3725	0.5648	0.0627	0.79102	0.18285	0.02612	0.79112	0.18283	0.02605	0.94528
15	0.2529	0.6244	0.1227	0.2526	0.6251	0.1224	0.67970	0.25582	0.06448	0.67934	0.25630	0.06437	0.93008
16	0.1956	0.6296	0.1748	0.1949	0.6309	0.1741	0.60045	0.29463	0.10491	0.59952	0.29578	0.10470	0.92160
17	0.1434	0.6245	0.2321	0.1429	0.6255	0.2316	0.50497	0.33524	0.15980	0.50394	0.33633	0.15973	0.91550
18	0.1113	0.6060	0.2827	0.1109	0.6065	0.2825	0.42981	0.35675	0.21345	0.42896	0.35746	0.21358	0.90986
19	0.0665	0.5324	0.4011	0.0660	0.5329	0.4010	0.29414	0.35899	0.34687	0.29257	0.36000	0.34743	0.89917
20	0.0503	0.4831	0.4666	0.0500	0.4832	0.4668	0.23377	0.34226	0.42397	0.23246	0.34282	0.42472	0.89400
21	0.0321	0.4036	0.5644	0.0319	0.4036	0.5645	0.15737	0.30163	0.54099	0.15670	0.30186	0.54144	0.88752
22	0.0141	0.2929	0.6930	0.0141	0.2927	0.6933	0.07259	0.22987	0.69754	0.07236	0.22971	0.69793	0.88013
23	0.00600	0.20271	0.79129	0.00598	0.20272	0.79130	0.03131	0.16127	0.80741	0.03121	0.16130	0.80749	0.87499
24	0.0012	0.1011	0.8976	0.0012	0.1012	0.8976	0.00625	0.08023	0.91353	0.00644	0.08025	0.91331	0.87032
25	0.00038	0	0.99962	0.00034	0	0.99966	0.00194	0.00000	0.99806	0.00194	0	0.99806	0.86691
26	n/a	n/a	n/a	0.0005 ^b	0	0.9995 ^b	n/a	n/a	n/a	0.00255	0	0.99745	n/a

^a Type B standard uncertainties u for temperature and pressure are $u(T)=0.03$ K and $u(p)=0.002$ MPa. The maximum error in density measurement is $5 \cdot 10^{-5}$ g/mL. For three-component samples (points # 2–24), combined standard uncertainties for mass fractions of H₂O, BEG, and TOL are 0.0008, 0.0008, and 0.0007, respectively. In case of the two-component sample (point 1) combined standard uncertainty for mass fractions of H₂O and TOL is 0.0004. For the two-component sample (point 25) combined standard uncertainty for mass fractions of H₂O and TOL are 0.0002.

^b Literature data on solubility of water in toluene [10].

Table 2Phase separation boundary on H₂O–BEG–TOL system at $T=293.15$ K, $p=0.100$ MPa and approximation residuals.

Point number I	One-phase points			Y residuals IV
	X II	Y III		
1	0.001	0		0.000823
2	0.0127	0.0207		-0.000372
3	0.0236	0.0402		-0.000548
4	0.0415	0.0711		-0.000329
5	0.0501	0.0855		-0.000290
6	0.0586	0.0994		-0.000291
7	0.0865	0.1452		0.000826
8	0.1186	0.1955		0.000963
9	0.1388	0.2254		-0.000419
10	0.1967	0.3141		0.000310
11	0.2185	0.3465		0.000549
12	0.2698	0.4153		-0.002843
13	0.3284	0.4918		0.000279
14	0.3985	0.5648		0.002594
15	0.5022	0.6251		0.000661
16	0.5653	0.6309		-0.004233
17	0.6286	0.6255		0.000472
18	0.6764	0.6065		0.002489
19	0.7708	0.5329		0.000522
20	0.818	0.4832		-0.000763
21	0.8848	0.4036		-0.001300
22	0.9695	0.2927		0.001037
23	1.0308	0.2027		0.000242
24	1.0949	0.1012		-0.000527
25	1.1541	0		0.000148

Y is mass fraction of hydrotrope ω_h , $X = (2 \times \omega_{TOL} + \omega_h) / \sqrt{3}$.

Y residuals is difference between experimental and fitted value (9th order polynomial) of mass fraction of hydrotrope.

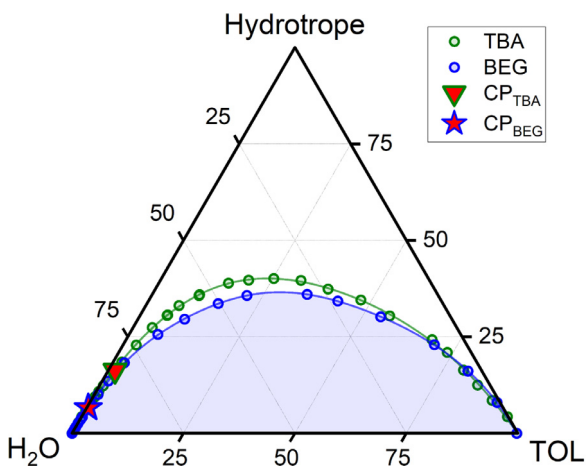


Fig. 3. Phase diagrams at 293.15 K of the systems W–BEG–TOL (this work) and W–TBA–TOL [6] in mole percentage; circles are experimental points (titration), color lines are 9th order polynomial approximations; red filled markers denote critical points; blue-filled area corresponds to the two-phase region in the W–BEG–TOL system. Data on W–BEG–TOL system are from Table 1 (x_{H_2O} is from Column XI; x_{BEG} is from Column XII; x_{TOL} is from Column XIII).

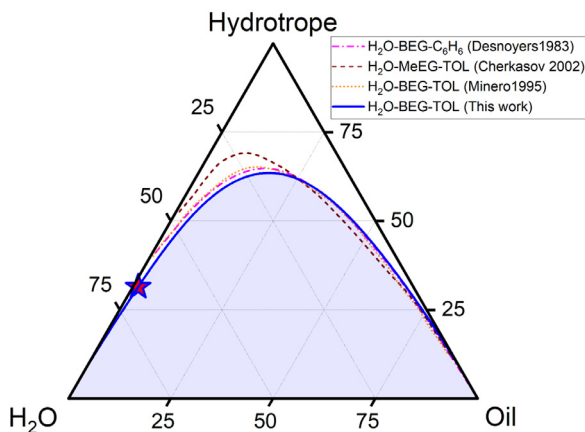


Fig. 4. Comparison of data of this work for the system W-BEG-TOL at 293.15 K with literature data for systems W-BEG-benzene at 298.15 K [7], W (pH=3)-BEG-toluene at 298.15 K [8], W-MeEG-toluene at 283.15 K [9] in mass percentage. Data on W-BEG-TOL system are from Table 1 (ω_{H_2O} is from Column V; ω_{BEG} is from Column VI; ω_{Tol} is from Column VII).

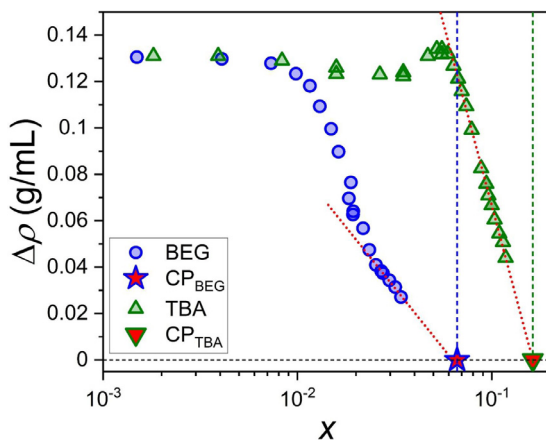


Fig. 5. Density difference of the equilibrated phases in the systems W-BEG-TOL (this work) and W-TBA-TOL [6] versus the equilibrium hydrotrope mole fraction in water phase at 293.15 K; red filled symbols are critical points, vertical color dashed lines are critical mole fractions of hydrotropes, red dotted lines are linear approximations of density difference for near-critical samples of W-BEG-TOL and W-TBA-TOL. Data on W-BEG-TOL system are from Tables 3,4 (X_{BEG} in water phase is from Table 3, Column VIII; $\Delta\rho$ is from Table 4, Column XVI).

Figs. 3 and 4 are in Table 1. Table 3 contains the compositions of the two-phase liquid samples, the interfacial tension between the equilibrated phases, and the normalized interfacial tension, which is illustrated by the interfacial tension isotherm shown in Fig. 6. Compositions, density, viscosity of the equilibrated phases, and density difference of the equilibrated phases are reported in Table 4. Fig. 5 shows density difference of the equilibrated phases for ternary systems water - BEG - toluene (Table 4) and water - TBA - toluene.

Table 3
Composition and interfacial tension for H₂O–BEG–TOL two-phase samples at 293.15 K.^a

Sample I	Initial composition						x_{BEG} in aqueous phase VIII	U_c of x_{BEG} in aqueous phase IX	ω_{BEG} in aqueous phase X	γ , 10^{-3} ·N/m XI	γ/γ_0 XII
	Mass fraction			Mole fraction							
	H ₂ O II	BEG III	TOL IV	H ₂ O V	BEG VI	TOL VII					
BEG0	0.5000	0	0.5000	0.8365	0.0000	0.1635	0	0	0.0000	34.5±0.3 (WP) ^b	1
BEG1	0.4927	0.0102	0.4971	0.8330	0.0026	0.1643	0.0015	0.00051	0.0097	18.70 ±0.02	5.421·10 ⁻¹
BEG2	0.4784	0.0302	0.4915	0.8261	0.0080	0.1660	0.0041	0.00061	0.0261	12.07±0.02	3.499·10 ⁻¹
BEG3	0.4417	0.0600	0.4983	0.8056	0.0167	0.1777	0.0073	0.00070	0.0461	8.97±0.01	2.601·10 ⁻¹
BEG4	0.4291	0.1200	0.4509	0.8012	0.0342	0.1646	0.0098	0.00078	0.0611	5.83±0.02	1.690·10 ⁻¹
BEG5	0.4251	0.1800	0.3949	0.8025	0.0518	0.1457	0.0116	0.00077	0.0714	4.225±0.006	1.225·10 ⁻¹
BEG6	0.4284	0.2600	0.3116	0.8099	0.0749	0.1152	0.0130	0.00076	0.0796	2.822±0.07	8.180·10 ⁻²
BEG7	0.4502	0.3200	0.2298	0.8277	0.0897	0.0826	0.0149	0.00089	0.0901	1.895±0.004	5.494·10 ⁻²
BEG8	0.4737	0.3600	0.1663	0.8442	0.0978	0.0579	0.0163	0.00063	0.0978	1.404±0.003	4.069·10 ⁻²
BEG9	0.5018	0.3901	0.1081	0.8616	0.1021	0.0363	0.0188	0.00039	0.1116	0.765±0.001	2.218·10 ⁻²
BEG10	0.5552	0.3701	0.0747	0.8866	0.0901	0.0233	0.0184	0.00039	0.1092	0.579±0.001	1.679·10 ⁻²
BEG11	0.5987	0.3477	0.0536	0.9041	0.0800	0.0158	0.0193	0.00039	0.1142	0.444±0.002	1.288·10 ⁻²
BEG12	0.6185	0.3300	0.0515	0.9111	0.0741	0.0148	0.0194	0.00035	0.1145	0.374±0.001	1.083·10 ⁻²
BEG13	0.6291	0.3304	0.0405	0.9152	0.0733	0.0115	0.0218	0.00034	0.1271	0.294±0.001	8.514·10 ⁻³
BEG14	0.6594	0.3133	0.0273	0.9255	0.0670	0.0075	0.0234	0.00032	0.1356	0.132±0.001	3.839·10 ⁻³
BEG15	0.6746	0.3047	0.0207	0.9304	0.0641	0.0056	0.0253	0.00031	0.1453	0.1194±0.0001	3.461·10 ⁻³
BEG16	0.6743	0.3055	0.0202	0.9303	0.0643	0.0054	0.0270	0.00038	0.1535	0.0481±0.0002	1.396·10 ⁻³
BEG17	0.6772	0.3032	0.0196	0.9312	0.0636	0.0053	0.0275	0.00032	0.1562	0.0426±0.0001	1.236·10 ⁻³
BEG18	0.6797	0.3018	0.0184	0.9320	0.0631	0.0049	0.0297	0.00036	0.1667	0.0236±0.0002	6.827·10 ⁻⁴
BEG19	0.6820	0.3005	0.0175	0.9327	0.0626	0.0047	0.0318	0.00034	0.1767	0.0234±0.0001	6.784·10 ⁻⁴
BEG20	0.6858	0.2984	0.0159	0.9338	0.0619	0.0042	0.0341	0.00037	0.1873	0.01241±0.00004	3.596·10 ⁻⁴

^a the standard deviation of interfacial tension is automatically calculated by Advance software (Krüss, Hamburg, Germany).

^b WP is the Wilhelmy plate method.

Table 4
Density ρ and dynamic viscosity η for equilibrated phases of H₂O–BEG–TOL two-phase samples at 293.15 K.^a

Sample I	Aqueous phase								Oil phase							
	Composition in mole fraction			U _c of composition in mole fraction		ρ , g/mL	η , mPa•s	Composition in mole fraction			U _c of composition in mole fraction		ρ , g/mL	η , mPa•s	$\Delta\rho$, g/mL	
	H ₂ O II	BEG III	TOL IV	BEG V	TOL VI			H ₂ O IX	BEG X	TOL XI	BEG XII	TOL XIII				
BEG0	rest	0	0.00011 ^c	n/a	0.000033 ^c	n/a	1.002 ^b	0.0024 ^c	0	0.9976 ^c	n/a	0.0008	n/a	0.588 ^b	n/a	
BEG1	rest	0	0.0002	n/a	0.0001	0.99819	1.002	0.0046	0	0.9954	n/a	0.0029	0.86691	0.588	0.13128	
BEG2	rest	0.0015	0.0002	0.0005	0.0001	0.99796	1.035	rest	0.0136	0.9839	0.0019	0.0030	0.86746	0.604	0.13050	
BEG3	rest	0.0041	0.0001	0.0006	0.0001	0.99757	1.092	rest	0.0300	0.9671	0.0095	0.0108	0.86780	0.613	0.12977	
BEG4	rest	0.0073	0.0001	0.0007	0.0001	0.99718	1.162	rest	0.0573	0.9389	0.0016	0.0029	0.86927	0.666	0.12791	
BEG5	rest	0.0098	0.0001	0.0008	0.0001	0.99690	1.226	rest	0.1384	0.8397	0.0015	0.0030	0.87352	0.772	0.12338	
BEG6	rest	0.0116	0.0001	0.0008	0.0001	0.99671	1.271	rest	0.2107	0.7313	0.0018	0.0036	0.87857	0.898	0.11814	
BEG7	rest	0.0130	0.0001	0.0008	0.0001	0.99655	1.321	rest	0.2995	0.5472	0.0028	0.0053	0.88723	1.286	0.10932	
BEG8	rest	0.0149	0.0002	0.0009	0.0002	0.99636	1.367	rest	0.3534	0.3822	0.0024	0.0038	0.89678	1.799	0.09958	
BEG9	rest	0.0163	0.0002	0.0007	0.0001	0.99618	1.415	rest	0.3640	0.2509	0.0019	0.0028	0.90640	2.442	0.08978	
BEG10	rest	0.0188	0.0003	0.0004	0.0001	0.99559	1.545	rest	0.3119	0.1246	0.0020	0.0016	0.91902	3.329	0.07657	
BEG11	rest	0.0184	0.0003	0.0004	0.0001	0.99571	1.486	rest	0.2746	0.0808	0.0015	0.0011	0.92603	3.791	0.06968	
BEG12	rest	0.0193	0.0003	0.0004	0.0001	0.99544	1.510	rest	0.2435	0.0553	0.0013	0.0008	0.93276	4.055	0.06268	
BEG13	rest	0.0194	0.0003	0.0004	0.0001	0.99542	1.511	rest	0.2504	0.0600	0.0013	0.0007	0.93132	4.062	0.06410	
BEG14	rest	0.0218	0.0004	0.0004	0.0001	0.99457	1.782	rest	0.2186	0.0412	0.0013	0.0008	0.93779	4.244	0.05678	
BEG15	rest	0.0234	0.0004	0.0003	0.0001	0.99390	1.732	rest	0.1776	0.0243	0.0011	0.0003	0.94641	4.053	0.04749	
BEG16	rest	0.0253	0.0005	0.0003	0.0001	0.99310	1.799	rest	0.1521	0.0170	0.0011	0.0004	0.95214	4.320	0.04096	
BEG17	rest	0.0270	0.0006	0.0004	0.0001	0.99240	1.845	rest	0.1436	0.0152	0.0011	0.0002	0.95406	4.304	0.03834	
BEG18	rest	0.0275	0.0006	0.0003	0.0001	0.99218	1.793	rest	0.1403	0.0145	0.0010	0.0002	0.95481	4.285	0.03737	
BEG19	rest	0.0297	0.0007	0.0004	0.0001	0.99126	1.902	rest	0.1310	0.0128	0.0010	0.0002	0.95692	4.225	0.03434	
BEG20	rest	0.0318	0.0009	0.0003	0.0001	0.99038	2.012	rest	0.1221	0.0113	0.0013	0.0002	0.95896	4.175	0.03142	
CP	rest	0.0341	0.0010	0.0004	0.0001	0.98940	1.910	rest	0.1090	0.0093	0.0009	0.0001	0.96227	4.117	0.02713	
CP	0.9301	0.0663	0.0036	0.0003	0.0001	0.97744	-	0.9301	0.0663	0.0036	0.0003	0.0001	0.97744	-	0	

^a the maximum error in density measurement is 5·10⁻⁵ g/mL, the maximum error is 0.5 % of the measured value for viscosity.

^b viscosity of pure water [11] and toluene [12].

^c literature data on solubility of toluene in water and water in toluene [10].

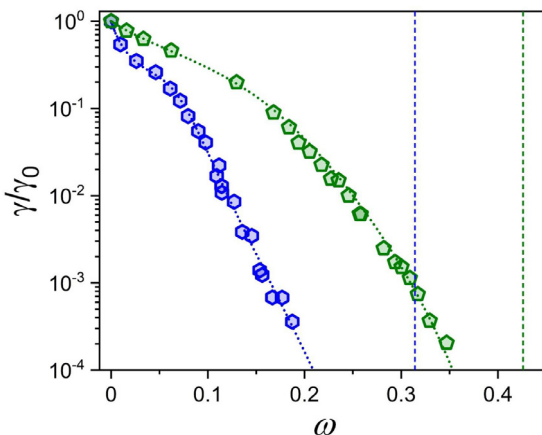


Fig. 6. Interfacial tension isotherms at 293.15 K for the W-BEG-TOL (this work) and W-TBA-TOL [6] systems versus the equilibrium hydrotrope mass fraction in water phase; the symbols are experimental data (green pentagons for TBA, blue hexagons for BEG), the dotted curves are crossover approximations [4], the vertical dashed lines indicate the critical hydrotrope concentrations. Data on W-BEG-TOL system are from Table 3 (ω_{BEG} in water phase is from Column X; γ/γ_0 is from Column XII).

2. Experimental Design, Materials and Methods

For the preparation of samples of the ternary system toluene (99.9% purity determined by the manufacturer, Ecos-1, Russia), BEG (99.5% purity determined by the manufacturer, Ecos-1, Russia), and deionized water ($\geq 18.1 \text{ M}\Omega\text{-cm}$, Simplicity UV, Millipore) were used. The samples were prepared in custom-made jacketed cells with an inverted ground joint using the freshly calibrated balances PA413C (resolution 0.001 g, maximum error $\pm 0.01 \text{ g}$, Ohaus, USA).

The location of the binodal curve and the critical point on the diagram was determined by volumetric titration from a two-phase state (detected visually as turbidity of the sample) to a homogeneous solution at $293.15 \pm 0.10 \text{ K}$. The position of the critical point was determined by titration with a volumetric phase ratio of 1:1. The samples were titrated in two stages. First, two-component water-toluene samples were titrated with BEG. Then, new two-phase samples with compositions in the immediate proximity to the expected separation boundary were prepared and titrated using small amounts of the titrants. The solubilities of toluene in water and water in toluene were obtained by titrating two-component samples with water or toluene. The combined standard uncertainty (U_c) was calculated according to JCGM 100:2008, taking into account the purity of the components, maximum errors of weighing, and dosing uncertainty of titrants [3]. The densities of homogeneous titrated samples were measured with density meter DMA 4500 (Anton Paar, Austria) to construct an interpolation of the density along the separation boundary. The maximum error in density measurement is $5 \cdot 10^{-5} \text{ g/mL}$.

The two-phase samples for density, viscosity, and interfacial tension measurements were magnetically stirred for at least 12 h at $293.15 \pm 0.1 \text{ K}$ after preparation, and then they were equilibrated without stirring for at least 12 h for complete stratification of phases. The density and dynamic viscosity of equilibrated phases in the two-phase region were measured at $293.15 \pm 0.03 \text{ K}$ using a rolling-ball viscometer Lovis 2000 ME (Anton Paar, Austria) integrated with a density meter DMA 4500. The maximum error is 0.5 % of the measured value for viscosity. The interfacial tension of two-phase samples was measured using a spinning drop tensiometer SDT (Krüss, Hamburg, Germany) equipped with a circulation thermostat, Ministat 230 (Huber, Offenburg, Germany). The interfacial tension between water and toluene was determined with a force tensiometer K20 (Krüss, Hamburg, Germany) equipped with a circulation thermostat, MPC-E (Huber, Offenburg, Germany), by the Wilhelmy plate method. The compositions of

equilibrated phases were obtained through density-interpolation data collected during titration. The interfacial tension data were approximated by a crossover function [4], combining the Langmuir – von Szyszkowski isotherm and the near-critical behavior predicted by the scaling theory [5].

Ethics Statements

The studies described in the manuscript were conducted adhering to Ethics in publishing standards (<https://www.elsevier.com/journals/data-in-brief/2352-3409/guide-for-authors>) and did not involve human or animal subjects.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Author Statement

Alexandra A. Kuchierskaya: Investigation, Data curation, Writing – original draft; **Anton P. Semenov:** Data curation, Visualization, Investigation, Writing – review & editing; **Adeliya R. Sayfutdinova:** Investigation; **Dmitry S. Kopitsyn:** Investigation; **Vladimir A. Vinokurov:** Supervision; **Mikhail A. Anisimov:** Supervision, Validation, Visualization, Writing – review & editing; **Andrei A. Novikov:** Supervision, Data curation, Validation, Writing – review & editing.

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References

- [1] A.A. Kuchierskaya, A.P. Semenov, A.R. Sayfutdinova, D.S. Kopitsyn, V.A. Vinokurov, M.A. Anisimov, A.A. Novikov, Interfacial tension and phase properties of water – hydrotrope – oil solutions: water –2-butoxyethanol – toluene, *J. Mol. Liq.* 344 (2021) 117683, doi:[10.1016/j.molliq.2021.117683](https://doi.org/10.1016/j.molliq.2021.117683).
- [2] A. Bazyleva, J. Abildskov, A. Anderko, O. Baudouin, Y. Chernyak, J.-C. de Hemptinne, V. Diky, R. Dohrn, J.R. Elliott, J. Jacquemin, J.-N. Jaubert, K.G. Joback, U.R. Kattner, G.M. Kontogeorgis, H. Loria, P.M. Mathias, J.P. O'Connell, W. Schröer, G.J. Smith, A. Soto, S. Wang, R.D. Weir, Good reporting practice for thermophysical and thermochemical property measurements (IUPAC Technical Report), *Pure Appl. Chem.* 93 (2021) 253–272, doi:[10.1515/pac-2020-0403](https://doi.org/10.1515/pac-2020-0403).
- [3] Joint Committee for Guides in Metrology. JCGM 100:2008, Evaluation of measurement data – guide to the expression of uncertainty in measurement, (2008).
- [4] A.A. Novikov, A.P. Semenov, V. Monje-Galvan, V.N. Kuryakov, J.B. Klauda, M.A. Anisimov, Dual action of hydrotropes at the water/oil interface, *J. Phys. Chem. C* 121 (2017) 16423–16431, doi:[10.1021/acs.jpcc.7b05156](https://doi.org/10.1021/acs.jpcc.7b05156).
- [5] J.S. Rowlinson, B. Widom, *Molecular Theory of Capillarity*, Oxford University Press, New York, 1989.
- [6] A.A. Novikov, A.P. Semenov, A.A. Kuchierskaya, D.S. Kopitsyn, V.A. Vinokurov, M.A. Anisimov, Generic nature of interfacial phenomena in solutions of nonionic hydrotropes, *Langmuir* 35 (41) (2019) 13480–13487, doi:[10.1021/acs.langmuir.9b02004](https://doi.org/10.1021/acs.langmuir.9b02004).
- [7] J.E. Desnoyers, F. Quirion, D. HÉTu, Gér. Perron, Tar sand extractions with microemulsions: I-the dissolution of light hydrocarbons by microemulsions using 2-butoxyethanol and diethylmethylamine as cosurfactants, *Can. J. Chem. Eng.* 61 (1983) 672–679, doi:[10.1002/cjce.5450610509](https://doi.org/10.1002/cjce.5450610509).
- [8] C. Minero, E. Pelizzetti, Reactivity and microstructure in water/ethoxy alcohols/toluene ternary solutions, *J. Dispers. Sci. Technol.* 16 (1995) 1–29, doi:[10.1080/01932699508943656](https://doi.org/10.1080/01932699508943656).
- [9] D.G. Cherkasov, K.K. Ilin, Liquid–liquid equilibrium and critical phenomena in the ternary system water + 2-methoxyethanol + toluene in the temperature range 283 K to 383 K, *J. Chem. Eng. Data* 47 (2002) 1303–1306, doi:[10.1021/je025544q](https://doi.org/10.1021/je025544q).

- [10] M. Goral, B. Wisniewska-Goclowaska, A. Skrzecz, I. Owczarek, K. Blazej, M.C. Haulait-Pirson, G.T. Hefter, F. Kapuku, Z. Maczynska, A. Szafranski, C.L. Young, IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater-revised and updated. Part 5. C7 hydrocarbons with water and heavy water, *J. Phys. Chem. Ref. Data* 34 (2005) 1399–1487, doi:[10.1063/1.1840737](https://doi.org/10.1063/1.1840737).
- [11] J. Kestin, M. Sokolov, W.A. Wakeham, Viscosity of liquid water in the range -8°C to 150°C , *J. Phys. Chem. Ref. Data* 7 (1978) 941–948, doi:[10.1063/1.555581](https://doi.org/10.1063/1.555581).
- [12] F.J.V. Santos, C.A. Nieto de Castro, J.H. Dymond, N.K. Dalaouti, M.J. Assael, A. Nagashima, Standard reference data for the viscosity of toluene, *J. Phys. Chem. Ref. Data* 35 (2006) 1–8, doi:[10.1063/1.1928233](https://doi.org/10.1063/1.1928233).