Appendix A. Supplementary material

Table S1. Experimental LLE data for DMSO (1)-aromatics (2)-decane (3) ternary system (mass fraction) at 30 °C under atmospheric pressure.[a]

DMSO phase			decane phase			K_{ar}	K_{al}
w_{11}	w_{12}	w_{13}	w_{21}	w_{22}	w_{23}		
DMSO (1) + *o*-xylene (2) + decane (3)							
0.9979	0.0000	0.0021	0.0053	0.0000	0.9947	—	—
0.9650	0.0261	0.0089	0.0074	0.0737	0.9189	0.3537	0.0097
0.9060	0.0826	0.0114	0.0120	0.2103	0.7777	0.3927	0.0147
0.8464	0.1390	0.0146	0.0167	0.3349	0.6484	0.4150	0.0226
0.7818	0.2004	0.0179	0.0314	0.4466	0.5220	0.4486	0.0342
0.7090	0.2670	0.0240	0.0586	0.5415	0.3999	0.4932	0.0599
0.6458	0.3153	0.0389	0.0786	0.5807	0.3407	0.5430	0.1140
0.6122	0.3427	0.0451	0.0876	0.5929	0.3196	0.5780	0.1412
DMSO (1) + *m*-xylene (2) + decane (3)							
0.9979	0.0000	0.0021	0.0053	0.0000	0.9947	—	—
0.9721	0.0211	0.0069	0.0080	0.0762	0.9157	0.2761	0.0075
0.9264	0.0660	0.0077	0.0134	0.2197	0.7669	0.3002	0.0100
0.8696	0.1184	0.0119	0.0222	0.3431	0.6347	0.3452	0.0188
0.8114	0.1713	0.0172	0.0346	0.4559	0.5095	0.3758	0.0338
0.7451	0.2315	0.0234	0.0556	0.5511	0.3933	0.4200	0.0596
0.6901	0.2759	0.0341	0.0728	0.5885	0.3387	0.4687	0.1006
0.6502	0.3037	0.0461	0.0790	0.6045	0.3164	0.5024	0.1457
DMSO (1) + *p*-xylene (2) + decane (3)							
0.9979	0.0000	0.0021	0.0053	0.0000	0.9947	—	—
0.9729	0.0204	0.0067	0.0057	0.0788	0.9155	0.2590	0.0074
0.9263	0.0649	0.0087	0.0096	0.2213	0.7691	0.2934	0.0114
0.8729	0.1145	0.0126	0.0141	0.3468	0.6391	0.3302	0.0196
0.8212	0.1650	0.0138	0.0280	0.4602	0.5118	0.3585	0.0270
0.7637	0.2200	0.0163	0.0485	0.5558	0.3957	0.3958	0.0413
0.7262	0.2537	0.0200	0.0664	0.5970	0.3366	0.4250	0.0595
0.7012	0.2721	0.0267	0.0730	0.6104	0.3166	0.4458	0.0844
DMSO (1) + ethylbenzene (2) + decane (3)							
0.9979	0.0000	0.0021	0.0053	0.0000	0.9947	—	—
0.9695	0.0248	0.0057	0.0076	0.0747	0.9177	0.3327	0.0062
0.9176	0.0750	0.0074	0.0135	0.2133	0.7733	0.3515	0.0096
0.8544	0.1349	0.0107	0.0169	0.3356	0.6475	0.4020	0.0165
0.7917	0.1942	0.0141	0.0318	0.4497	0.5185	0.4318	0.0272
0.7193	0.2605	0.0202	0.0577	0.5428	0.3995	0.4799	0.0506
0.6732	0.3016	0.0251	0.0785	0.5787	0.3428	0.5212	0.0734
0.6544	0.3184	0.0273	0.0898	0.5926	0.3176	0.5373	0.0858

a Model oils were prepared using a Sartorius BSA124S analytical balance (d=0.1 mg). The standard uncertainties: u(T) = 0.05 °C, u(p) = 0.1 MPa.

Table S2. The fitting parameters *a*, *b*, and corresponding linear regression coefficients R^2 of Othmer-Tobias equation for DMSO-aromatics-decane experimental data.

LLE	*a*	*b*	R^2
DMSO (1) + *o*-xylene (2) + decane (3)	0.9324	-1.174	0.9984
DMSO (1) + *m*-xylene (2) + decane (3)	0.9067	-1.4062	0.9994
DMSO (1) + *p*-xylene (2) + decane (3)	0.8778	-1.508	0.9993
DMSO (1) + ethylbenzene (2) + decane (3)	0.9185	-1.2897	0.9994

Table S3. Interaction energies (kJ/mol) of stationary interaction dimers calculated at M06-2X/6-311++g(d, p) level.

	o-xylene	*m*-xylene	*p*-xylene	ethylbenzene
DMSO	-37.7982	-32.3148	-30.3056	-32.7752
decane	-29.6358	-31.6450	-30.1800	-30.0544
decane(DMSO)	-21.8316	-23.2202	-20.5230	-21.0035

Table S4. AIM topological analysis properties at (3,-1) BCP of aromatics-DMSO dimers.

	Bond paths	ρ(r)/a.u.	$\nabla^2\rho$(r)/a.u.	Distance/Å	*H*(r)/a.u.	E_H(kJ/mol)
o-xylene/DMSO	C_{11}-H_{12}⋯O_{19}(58)	0.0131	0.0413	2.350	＞0	-2.18
	C_{15}-H_{16}⋯O_{19}(62)	0.0129	0.0436	2.306	＞0	-2.14
	C_4⋯H_{23}-C_{20}(41)	0.0066	0.0194	2.810		
	C_2⋯H_{25}-C_{24}(45)	0.0073	0.0250	2.800	＞0	-0.89
m-xylene/DMSO	C_{11}-H_{14}⋯O_{19}(60)	0.0122	0.0407	2.348	＞0	-1.98
	C_2⋯S_{28}(49)	0.0081	0.0264	3.283		
	C_4⋯H_{21}-C_{20}(50)	0.0077	0.0257	2.721	＞0	-0.98
p-xylene/DMSO	C_{11}-H_{13}⋯O_{19}(58)	0.0131	0.0417	2.348	＞0	-2.18
	C_5⋯O_{19}(52)	0.0071	0.0232	3.225		
	C_5⋯H_{25}-C_{24}(41)	0.0074	0.0255	2.782	＞0	-0.91
	C_6⋯H_{23}-C_{20}(50)	0.0064	0.0193	2.833		
ethybenzene/DMSO	C_{15}-H_{17}⋯O_{19}(60)	0.0097	0.0367	2.443	＞0	-1.42
	C_{12}-H_{13}⋯O_{19}(59)	0.0097	0.0354	2.561	＞0	-1.42
	C_3⋯O_{19}(54)	0.0071	0.0223	3.262		
	C_2⋯H_{23}-C_{20}(37)	0.0058	0.0170	2.876		
	C_3⋯H_{25}-C_{24}(47)	0.0075	0.0256	2.771	＞0	-0.93

Table S5. AIM topological analysis properties at (3,-1) BCP of aromatics-decane dimers.

	Bond paths	ρ(r)/a.u.	$\nabla^2\rho$(r)/a.u.	Distance/Å
o-xylene/decane	$C_6\cdots H_{28}$-C_{26}(93)	0.0057	0.0168	2.920
	$C_1\cdots H_{31}$-C_{29}(82)	0.0065	0.0194	2.907
	$C_2\cdots H_{33}$-C_{32}(95)	0.0062	0.0202	2.966
	$C_3\cdots H_{37}$-C_{35}(120)	0.0053	0.0161	3.052
	C_{15}-$H_{16}\cdots H_{37}$-C_{35}(77)	0.0065	0.0223	2.276
	C_{11}-$H_{12}\cdots H_{37}$-C_{35}(86)	0.0066	0.0232	2.309
	C_{11}-$H_{12}\cdots H_{43}$-C_{41}(89)	0.0062	0.0218	2.311
	$C_3\cdots H_{39}$-C_{38}(102)	0.0060	0.0185	2.904
	$C_{11}\cdots H_{39}$-C_{38}(99)	0.0058	0.0212	2.877
m-xylene/decane	C_{15}-$H_{18}\cdots H_{48}$-C_{47}(92)	0.0050	0.0176	2.531
	C_{15}-$H_{18}\cdots H_{46}$-C_{44}(79)	0.0055	0.0199	2.459
	C_{15}-$H_{16}\cdots H_{42}$-C_{41}(93)	0.0053	0.0187	2.477
	$C_1\cdots H_{42}$-C_{41}(88)	0.0059	0.0179	2.950
	$C_6\cdots H_{46}$-C_{44}(73)	0.0055	0.0163	2.943
	$C_6\cdots H_{40}$-C_{38}(69)	0.0060	0.0195	2.912
	$C_2\cdots H_{40}$-C_{38}(78)	0.0061	0.0196	2.974
	$C_3\cdots H_{36}$-C_{35}(86)	0.0060	0.0178	2.963
	$C_3\cdots H_{34}$-C_{32}(70)	0.0059	0.0176	2.943
	C_{11}-$H_{13}\cdots H_{30}$-C_{29}(84)	0.0055	0.0193	2.526
p-xylene/decane	$C_{11}\cdots H_{48}$-C_{47}(84)	0.0058	0.0215	2.870
	C_{11}-$H_{13}\cdots H_{46}$-C_{44}(93)	0.0050	0.0184	2.455
	$C_5\cdots H_{46}$-C_{44}(83)	0.0059	0.0175	2.912
	$C_1\cdots H_{42}$-C_{41}(79)	0.0064	0.0203	2.864
	$C_4\cdots H_{40}$-C_{38}(81)	0.0070	0.0215	2.805
	$C_3\cdots H_{36}$-C_{35}(76)	0.0066	0.0218	2.800
	C_4-$H_9\cdots H_{34}$-C_{32}(71)	0.0032	0.0101	2.695
	C_{15}-$H_{18}\cdots H_{34}$-C_{32}(72)	0.0044	0.0153	2.547
	C_{15}-$H_{18}\cdots H_{30}$-C_{29}(73)	0.0046	0.0158	2.522
ethybenzene/decane	C_{15}-$H_{18}\cdots H_{25}$-C_{23}(99)	0.0060	0.0211	2.325
	C_{15}-$H_{18}\cdots H_{27}$-C_{26}(103)	0.0056	0.0204	2.583
	C_{15}-$H_{18}\cdots H_{30}$-C_{29}(98)	0.0065	0.0228	2.312
	C_{12}-$H_{14}\cdots H_{27}$-C_{26}(102)	0.0071	0.0250	2.257
	C_{12}-$H_{14}\cdots H_{34}$-C_{32}(95)	0.0072	0.0254	2.237
	$C_3\cdots H_{30}$-C_{29}(101)	0.0055	0.0158	2.962
	$C_4\cdots H_{34}$-C_{32}(97)	0.0054	0.0162	3.034
	$C_6\cdots H_{36}$-C_{35}(89)	0.0063	0.0207	2.908
	$C_6\cdots H_{40}$-C_{38}(88)	0.0061	0.0182	2.942
	$C_6\cdots H_{42}$-C_{41}(86)	0.0056	0.0166	2.953

Table S6. Contribution percentage of the energy decomposition derived dispersion, electrostatic, and induction attractive effects within aromatics-DMSO dimers at SAPT2+(3)δMP2/aug-cc-pVTZ level.

	Attraction		
	E_{dis}%	E_{elst}%	E_{ind}%
o-xylene/DMSO	49.57	37.83	12.60
m-xylene/DMSO	50.52	37.21	12.27
p-xylene/DMSO	53.14	35.57	11.29
ethylbenzene/DMSO	53.30	35.49	11.21

Table S7. Contribution percentage of the energy decomposition derived dispersion, electrostatic, and induction attractive effects within aromatics-decane dimers at SAPT2+(3)δMP2/aug-cc-pVTZ level.

	Attraction		
	E_{dis}%	E_{elst}%	E_{ind}%
o-xylene/decane	70.89	23.42	5.69
m-xylene/decane	70.93	23.91	5.16
p-xylene/decane	70.56	24.29	5.15
ethylbenzene/decane	70.41	23.79	5.80