

Study of Properties and Structure of Aromatic Ester Solvents

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Supporting Information

Table S1. Experimental Density, ρ (g cm^{-3}), of Pure Solvents as a Function of Pressure and Temperature

P (MPa)	$T(\text{K})$								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
MB									
0.10	1.1015	1.0921	1.0827	1.0730	1.0633	1.0536	1.0441	1.0344	1.0249
1.00	1.1021	1.0926	1.0832	1.0736	1.0638	1.0543	1.0448	1.0351	1.0256
5.00	1.1044	1.0950	1.0858	1.0762	1.0667	1.0572	1.0480	1.0384	1.0291
10.00	1.1072	1.0979	1.0890	1.0795	1.0701	1.0608	1.0517	1.0424	1.0333
15.00	1.1099	1.1008	1.0918	1.0826	1.0734	1.0643	1.0553	1.0462	1.0373
20.00	1.1126	1.1036	1.0948	1.0857	1.0766	1.0676	1.0588	1.0498	1.0412
25.00	1.1152	1.1063	1.0976	1.0886	1.0797	1.0709	1.0622	1.0534	1.0449
30.00	1.1177	1.1090	1.1004	1.0915	1.0828	1.0740	1.0655	1.0569	1.0485
35.00	1.1202	1.1116	1.1031	1.0943	1.0857	1.0771	1.0688	1.0603	1.0520
40.00	1.1227	1.1141	1.1057	1.0971	1.0886	1.0801	1.0719	1.0635	1.0554
45.00	1.1251	1.1166	1.1083	1.0998	1.0914	1.0830	1.0749	1.0667	1.0587
50.00	1.1274	1.1191	1.1109	1.1024	1.0941	1.0859	1.0779	1.0698	1.0619
55.00	1.1297	1.1214	1.1134	1.1050	1.0968	1.0887	1.0808	1.0728	1.0651
60.00	1.1318	1.1236	1.1156	1.1074	1.0993	1.0912	1.0835	1.0755	1.0679
EB									
0.10	1.0594	1.0503	1.0409	1.0316	1.0221	1.0128	1.0034	0.9941	0.9842
1.00	1.0599	1.0508	1.0415	1.0322	1.0228	1.0135	1.0042	0.9949	0.9850
5.00	1.0623	1.0534	1.0442	1.0350	1.0258	1.0166	1.0075	0.9983	0.9886
10.00	1.0652	1.0564	1.0474	1.0384	1.0293	1.0204	1.0113	1.0024	0.9930
15.00	1.0680	1.0594	1.0505	1.0416	1.0327	1.0239	1.0151	1.0064	0.9971
20.00	1.0708	1.0623	1.0535	1.0447	1.0360	1.0274	1.0188	1.0102	1.0011
25.00	1.0735	1.0651	1.0565	1.0478	1.0392	1.0307	1.0222	1.0138	1.0050
30.00	1.0761	1.0678	1.0593	1.0508	1.0423	1.0340	1.0256	1.0174	1.0087
35.00	1.0787	1.0705	1.0621	1.0537	1.0454	1.0371	1.0289	1.0208	1.0123
40.00	1.0812	1.0732	1.0648	1.0565	1.0483	1.0402	1.0321	1.0241	1.0158
45.00	1.0837	1.0758	1.0675	1.0593	1.0512	1.0432	1.0353	1.0274	1.0192
50.00	1.0861	1.0783	1.0701	1.0620	1.0540	1.0461	1.0383	1.0306	1.0225
55.00	1.0885	1.0807	1.0726	1.0646	1.0567	1.0489	1.0412	1.0336	1.0256
60.00	1.0908	1.0831	1.0750	1.0671	1.0592	1.0516	1.0440	1.0363	1.0285
PB									
0.10	1.0339	1.0251	1.0160	1.0070	0.9982	0.9891	0.9800	0.9713	0.9621
1.00	1.0344	1.0256	1.0166	1.0076	0.9989	0.9898	0.9808	0.9720	0.9629
5.00	1.0368	1.0281	1.0192	1.0104	1.0017	0.9928	0.9840	0.9753	0.9664
10.00	1.0397	1.0311	1.0223	1.0137	1.0052	0.9965	0.9878	0.9794	0.9707
15.00	1.0425	1.0341	1.0254	1.0169	1.0086	1.0000	0.9916	0.9832	0.9748
20.00	1.0452	1.0369	1.0284	1.0200	1.0118	1.0034	0.9951	0.9870	0.9787
25.00	1.0479	1.0397	1.0313	1.0230	1.0150	1.0067	0.9985	0.9906	0.9824
30.00	1.0505	1.0424	1.0341	1.0259	1.0180	1.0099	1.0019	0.9941	0.9861
35.00	1.0530	1.0451	1.0369	1.0288	1.0210	1.0130	1.0051	0.9975	0.9896
40.00	1.0555	1.0477	1.0396	1.0316	1.0239	1.0160	1.0083	1.0007	0.9930
45.00	1.0580	1.0502	1.0422	1.0343	1.0267	1.0190	1.0113	1.0039	0.9963
50.00	1.0604	1.0527	1.0448	1.0370	1.0295	1.0219	1.0143	1.0070	0.9994
55.00	1.0627	1.0551	1.0473	1.0396	1.0322	1.0246	1.0172	1.0100	1.0025
60.00	1.0649	1.0573	1.0498	1.0420	1.0347	1.0274	1.0200	1.0127	1.0054

Table S1. Continued

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
BB									
0.10	1.0176	1.0091	1.0005	0.9920	0.9834	0.9747	0.9662	0.9579	0.9495
1.00	1.0182	1.0097	1.0010	0.9926	0.9840	0.9754	0.9669	0.9586	0.9502
5.00	1.0205	1.0121	1.0035	0.9953	0.9868	0.9784	0.9701	0.9619	0.9537
10.00	1.0233	1.0151	1.0067	0.9986	0.9902	0.9820	0.9738	0.9658	0.9578
15.00	1.0261	1.0179	1.0097	1.0018	0.9936	0.9854	0.9775	0.9696	0.9618
20.00	1.0288	1.0208	1.0126	1.0048	0.9968	0.9888	0.9810	0.9732	0.9657
25.00	1.0314	1.0235	1.0155	1.0077	0.9998	0.9920	0.9843	0.9767	0.9694
30.00	1.0340	1.0262	1.0182	1.0106	1.0028	0.9951	0.9876	0.9801	0.9728
35.00	1.0365	1.0288	1.0210	1.0134	1.0058	0.9982	0.9908	0.9834	0.9763
40.00	1.0390	1.0313	1.0236	1.0162	1.0086	1.0011	0.9939	0.9866	0.9797
45.00	1.0414	1.0338	1.0262	1.0189	1.0114	1.0040	0.9969	0.9897	0.9829
50.00	1.0437	1.0363	1.0287	1.0215	1.0141	1.0068	0.9998	0.9928	0.9860
55.00	1.0460	1.0386	1.0312	1.0240	1.0168	1.0095	1.0026	0.9957	0.9890
60.00	1.0482	1.0408	1.0335	1.0264	1.0193	1.0121	1.0053	0.9986	0.9919
PA									
0.10	1.0903	1.0805	1.0706	1.0604	1.0504	1.0405	1.0305	1.0204	1.0104
1.00	1.0907	1.0809	1.0712	1.0608	1.0510	1.0411	1.0312	1.0210	1.0111
5.00	1.0929	1.0833	1.0738	1.0635	1.0538	1.0441	1.0343	1.0245	1.0146
10.00	1.0957	1.0862	1.0768	1.0667	1.0573	1.0477	1.0381	1.0285	1.0188
15.00	1.0984	1.0891	1.0797	1.0699	1.0606	1.0512	1.0418	1.0323	1.0229
20.00	1.1011	1.0919	1.0827	1.0729	1.0638	1.0546	1.0453	1.0361	1.0268
25.00	1.1036	1.0946	1.0855	1.0759	1.0669	1.0578	1.0487	1.0397	1.0306
30.00	1.1062	1.0972	1.0883	1.0788	1.0699	1.0610	1.0520	1.0432	1.0342
35.00	1.1087	1.0998	1.0910	1.0817	1.0729	1.0641	1.0553	1.0465	1.0378
40.00	1.1111	1.1024	1.0936	1.0845	1.0758	1.0671	1.0584	1.0499	1.0412
45.00	1.1135	1.1049	1.0962	1.0872	1.0786	1.0701	1.0615	1.0530	1.0445
50.00	1.1158	1.1073	1.0987	1.0898	1.0813	1.0729	1.0644	1.0562	1.0478
55.00	1.1181	1.1097	1.1012	1.0924	1.0840	1.0757	1.0674	1.0592	1.0508
60.00	1.1202	1.1119	1.1036	1.0948	1.0866	1.0782	1.0702	1.0621	1.0540
MS									
0.10	1.1958	1.1862	1.1765	1.1671	1.1573	1.1475	1.1376	1.1274	1.1172
1.00	1.1963	1.1867	1.1771	1.1677	1.1579	1.1481	1.1382	1.1282	1.1180
5.00	1.1985	1.1891	1.1795	1.1702	1.1606	1.1510	1.1412	1.1313	1.1213
10.00	1.2012	1.1919	1.1825	1.1734	1.1639	1.1544	1.1448	1.1351	1.1253
15.00	1.2039	1.1947	1.1854	1.1764	1.1671	1.1578	1.1483	1.1388	1.1292
20.00	1.2065	1.1974	1.1883	1.1794	1.1702	1.1611	1.1517	1.1424	1.1329
25.00	1.2090	1.2001	1.1911	1.1823	1.1732	1.1642	1.1550	1.1458	1.1366
30.00	1.2115	1.2027	1.1938	1.1851	1.1762	1.1673	1.1583	1.1492	1.1401
35.00	1.2140	1.2052	1.1964	1.1879	1.1791	1.1703	1.1614	1.1525	1.1435
40.00	1.2164	1.2077	1.1990	1.1906	1.1819	1.1732	1.1644	1.1556	1.1468
45.00	1.2187	1.2102	1.2016	1.1932	1.1847	1.1761	1.1674	1.1587	1.1500
50.00	1.2210	1.2126	1.2041	1.1959	1.1873	1.1789	1.1704	1.1618	1.1532
55.00	1.2233	1.2150	1.2066	1.1984	1.1900	1.1817	1.1732	1.1647	1.1563
60.00	1.2254	1.2172	1.2089	1.2008	1.1924	1.1842	1.1760	1.1674	1.1593

Table S2. Fitting Parameters of the TRIDEN Correlation of Density (g cm^{-3}) with Pressure and Temperature, eqs. 2 - 4, and AAD values for Pure Solvents. The Parameters are applicable within 278.15 – 358.15 K and 0.1 – 60 MPa ranges

Parameter	MB	EB	PB	BB	PA	MS
C_T	0.091502	0.083735	0.083046	0.082852	0.086330	0.081130
$b_0(\text{MPa})$	286.484	274.841	273.127	277.275	276.393	304.543
$b_1(\text{MPa})$	-1.3656	-23.9139	-44.8804	-62.4779	-9.1679	13.7794
$b_2(\text{MPa})$	-17.3213	-9.5596	3.4904	13.0039	-12.3291	-31.9487
$b_3(\text{MPa})$	0.49646	0.49260	-1.18874	-2.30534	0.13121	3.60509
$E_T(\text{K})$	106.45	99.26	93.59	88.99	100.97	98.47
$A_R(\text{g cm}^{-3})$	45.9026	68.3336	93.9734	131.4046	57.0405	56.3027
B_R	5.911766	7.335465	8.707325	10.380903	6.591603	6.312095
$C_R(\text{K})$	819.963	842.495	884.845	963.139	829.005	838.620
D_R	-0.228246	-0.217666	-0.213754	-0.219019	-0.230400	-0.215635
AAD	0.0175	0.0138	0.0147	0.0144	0.0164	0.0066

Table S3. Isobaric Expansivity, α_p (kK⁻¹) of Pure Solvents as a Function of Pressure and Temperature

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
	MB								
0.10	0.823	0.842	0.862	0.882	0.904	0.927	0.950	0.975	1.001
1.00	0.821	0.839	0.859	0.879	0.901	0.923	0.946	0.969	0.994
5.00	0.812	0.829	0.847	0.866	0.885	0.905	0.925	0.945	0.964
10.00	0.801	0.817	0.834	0.850	0.867	0.884	0.900	0.915	0.929
15.00	0.791	0.806	0.821	0.836	0.850	0.864	0.877	0.888	0.897
20.00	0.781	0.795	0.808	0.822	0.834	0.846	0.856	0.863	0.867
25.00	0.771	0.784	0.796	0.808	0.819	0.828	0.836	0.840	0.839
30.00	0.762	0.774	0.785	0.796	0.805	0.812	0.817	0.818	0.813
35.00	0.754	0.765	0.775	0.784	0.791	0.796	0.799	0.797	0.789
40.00	0.746	0.755	0.764	0.772	0.778	0.782	0.782	0.777	0.766
45.00	0.738	0.747	0.755	0.761	0.766	0.768	0.766	0.759	0.744
50.00	0.730	0.738	0.745	0.751	0.754	0.754	0.751	0.742	0.724
55.00	0.723	0.730	0.736	0.741	0.743	0.742	0.736	0.725	0.705
60.00	0.716	0.723	0.728	0.731	0.732	0.730	0.723	0.709	0.687
	EB								
0.10	0.839	0.857	0.876	0.896	0.917	0.939	0.962	0.985	1.010
1.00	0.836	0.854	0.873	0.893	0.913	0.934	0.956	0.979	1.003
5.00	0.826	0.843	0.860	0.878	0.897	0.915	0.934	0.953	0.972
10.00	0.814	0.829	0.845	0.861	0.877	0.893	0.909	0.924	0.937
15.00	0.802	0.816	0.831	0.845	0.859	0.872	0.885	0.896	0.905
20.00	0.791	0.804	0.817	0.830	0.842	0.853	0.863	0.871	0.876
25.00	0.781	0.793	0.805	0.816	0.826	0.835	0.843	0.848	0.849
30.00	0.771	0.782	0.793	0.802	0.811	0.819	0.824	0.826	0.824
35.00	0.762	0.772	0.781	0.790	0.797	0.803	0.806	0.806	0.801
40.00	0.753	0.762	0.771	0.778	0.784	0.788	0.790	0.787	0.780
45.00	0.744	0.753	0.760	0.767	0.772	0.774	0.774	0.770	0.760
50.00	0.736	0.744	0.751	0.756	0.760	0.761	0.760	0.753	0.741
55.00	0.729	0.736	0.742	0.746	0.749	0.749	0.746	0.738	0.724
60.00	0.721	0.728	0.733	0.737	0.738	0.737	0.733	0.723	0.708
	PB								
0.10	0.827	0.843	0.861	0.879	0.898	0.918	0.938	0.959	0.981
1.00	0.824	0.841	0.858	0.876	0.894	0.913	0.933	0.953	0.974
5.00	0.815	0.830	0.846	0.862	0.878	0.894	0.911	0.927	0.942
10.00	0.803	0.817	0.831	0.845	0.859	0.872	0.885	0.896	0.906
15.00	0.792	0.805	0.817	0.830	0.841	0.852	0.862	0.869	0.873
20.00	0.782	0.793	0.805	0.815	0.825	0.834	0.840	0.843	0.842
25.00	0.772	0.783	0.793	0.802	0.810	0.816	0.820	0.820	0.815
30.00	0.763	0.773	0.781	0.789	0.796	0.800	0.801	0.798	0.789
35.00	0.754	0.763	0.771	0.777	0.782	0.784	0.784	0.778	0.765
40.00	0.746	0.754	0.761	0.766	0.769	0.770	0.767	0.759	0.743
45.00	0.738	0.745	0.751	0.755	0.757	0.757	0.752	0.741	0.723
50.00	0.731	0.737	0.742	0.745	0.746	0.744	0.737	0.725	0.704
55.00	0.724	0.729	0.733	0.736	0.736	0.732	0.724	0.709	0.686
60.00	0.717	0.722	0.725	0.727	0.725	0.721	0.711	0.695	0.669

Table S3. Continued

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
BB									
0.10	0.806	0.821	0.836	0.851	0.868	0.884	0.901	0.919	0.938
1.00	0.804	0.818	0.833	0.848	0.864	0.880	0.896	0.913	0.930
5.00	0.795	0.808	0.821	0.835	0.848	0.862	0.874	0.887	0.897
10.00	0.784	0.796	0.808	0.819	0.830	0.840	0.849	0.856	0.860
15.00	0.774	0.785	0.795	0.804	0.813	0.820	0.826	0.828	0.825
20.00	0.765	0.774	0.783	0.791	0.797	0.802	0.804	0.802	0.794
25.00	0.756	0.764	0.772	0.778	0.783	0.785	0.784	0.778	0.766
30.00	0.747	0.755	0.761	0.766	0.769	0.769	0.765	0.756	0.739
35.00	0.739	0.746	0.751	0.754	0.756	0.754	0.748	0.736	0.715
40.00	0.732	0.737	0.741	0.744	0.744	0.740	0.732	0.717	0.692
45.00	0.724	0.729	0.732	0.733	0.732	0.727	0.716	0.699	0.671
50.00	0.717	0.721	0.724	0.724	0.721	0.714	0.702	0.682	0.651
55.00	0.711	0.714	0.716	0.715	0.711	0.703	0.688	0.666	0.632
60.00	0.704	0.707	0.708	0.706	0.701	0.691	0.676	0.651	0.615
PA									
0.10	0.867	0.886	0.907	0.928	0.951	0.974	0.999	1.024	1.051
1.00	0.864	0.884	0.904	0.925	0.947	0.970	0.993	1.018	1.043
5.00	0.855	0.873	0.892	0.911	0.931	0.951	0.971	0.991	1.010
10.00	0.844	0.860	0.877	0.894	0.912	0.928	0.945	0.960	0.972
15.00	0.833	0.848	0.864	0.879	0.894	0.908	0.920	0.931	0.937
20.00	0.823	0.837	0.851	0.864	0.877	0.888	0.897	0.904	0.905
25.00	0.813	0.826	0.838	0.850	0.861	0.870	0.876	0.879	0.875
30.00	0.804	0.816	0.827	0.837	0.846	0.853	0.856	0.855	0.848
35.00	0.795	0.806	0.816	0.825	0.832	0.837	0.838	0.834	0.822
40.00	0.786	0.796	0.805	0.813	0.818	0.821	0.820	0.813	0.798
45.00	0.778	0.787	0.795	0.802	0.806	0.807	0.804	0.794	0.776
50.00	0.771	0.779	0.786	0.791	0.794	0.793	0.788	0.776	0.755
55.00	0.763	0.771	0.777	0.781	0.782	0.780	0.773	0.759	0.735
60.00	0.756	0.763	0.768	0.771	0.771	0.768	0.759	0.743	0.716
MS									
0.10	0.773	0.790	0.808	0.827	0.846	0.866	0.887	0.909	0.932
1.00	0.771	0.788	0.806	0.824	0.843	0.863	0.883	0.905	0.927
5.00	0.762	0.778	0.795	0.812	0.830	0.848	0.867	0.886	0.906
10.00	0.752	0.767	0.782	0.798	0.814	0.830	0.847	0.864	0.882
15.00	0.742	0.755	0.770	0.784	0.799	0.814	0.829	0.844	0.859
20.00	0.732	0.745	0.758	0.771	0.785	0.798	0.812	0.825	0.838
25.00	0.723	0.735	0.747	0.759	0.772	0.784	0.795	0.807	0.818
30.00	0.714	0.725	0.737	0.748	0.759	0.770	0.780	0.790	0.800
35.00	0.706	0.716	0.727	0.737	0.747	0.757	0.766	0.775	0.782
40.00	0.698	0.708	0.717	0.727	0.736	0.745	0.753	0.760	0.766
45.00	0.690	0.699	0.708	0.717	0.725	0.733	0.740	0.746	0.751
50.00	0.683	0.691	0.700	0.708	0.715	0.722	0.728	0.733	0.737
55.00	0.676	0.684	0.691	0.699	0.705	0.711	0.717	0.721	0.724
60.00	0.669	0.676	0.684	0.690	0.696	0.701	0.706	0.709	0.711

Table S4 Isothermal Compressibility, κ_T (TPa⁻¹), of Pure Solvents as a Function of Pressure and Temperature

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
MB									
0.10	527.1	551.8	579.9	611.9	648.8	691.5	741.7	801.2	872.9
1.00	524.6	549.1	576.9	608.6	645.0	687.3	736.8	795.5	866.1
5.00	513.9	537.4	564.0	594.3	629.0	669.1	715.9	771.2	837.4
10.00	501.2	523.5	548.7	577.3	610.0	647.7	691.4	742.9	804.2
15.00	489.1	510.3	534.3	561.4	592.2	627.7	668.7	716.8	773.7
20.00	477.6	497.9	520.6	546.3	575.5	608.9	647.5	692.5	745.5
25.00	466.7	486.0	507.7	532.1	559.8	591.3	627.7	669.9	719.4
30.00	456.3	474.7	495.4	518.6	544.9	574.8	609.1	648.7	695.1
35.00	446.3	464.0	483.7	505.9	530.8	559.2	591.6	629.0	672.6
40.00	436.8	453.7	472.6	493.7	517.5	544.4	575.2	610.5	651.5
45.00	427.8	444.0	462.0	482.2	504.9	530.5	559.7	593.1	631.7
50.00	419.1	434.6	451.9	471.2	492.9	517.3	545.0	576.7	613.2
55.00	410.8	425.7	442.3	460.8	481.5	504.8	531.2	561.2	595.8
60.00	402.8	417.2	433.1	450.8	470.6	492.9	518.0	546.6	579.4
EB									
0.10	582.7	611.2	643.1	679.1	720.0	766.8	820.9	884.0	958.7
1.00	579.4	607.5	639.0	674.6	714.9	761.0	814.3	876.4	949.7
5.00	565.1	591.8	621.7	655.3	693.2	736.6	786.3	844.1	912.0
10.00	548.2	573.3	601.3	632.7	668.1	708.2	754.1	807.1	868.9
15.00	532.4	556.0	582.3	611.7	644.7	682.0	724.5	773.3	829.9
20.00	517.4	539.8	564.5	592.1	623.0	657.8	697.3	742.4	794.5
25.00	503.4	524.5	547.9	573.8	602.8	635.3	672.1	714.0	762.0
30.00	490.1	510.1	532.2	556.7	583.9	614.4	648.8	687.7	732.3
35.00	477.5	496.5	517.4	540.5	566.2	594.9	627.1	663.4	704.8
40.00	465.6	483.7	503.5	525.4	549.6	576.6	606.8	640.9	679.5
45.00	454.3	471.5	490.3	511.1	534.0	559.5	587.9	619.9	656.0
50.00	443.6	460.0	477.9	497.6	519.3	543.4	570.2	600.3	634.1
55.00	433.4	449.0	466.1	484.8	505.5	528.3	553.6	581.9	613.7
60.00	423.6	438.6	454.9	472.7	492.3	514.0	538.0	564.7	594.7
PB									
0.10	595.5	622.4	652.7	687.1	726.6	772.3	825.8	889.4	966.0
1.00	592.0	618.5	648.5	682.5	721.4	766.4	819.1	881.6	956.8
5.00	576.9	602.1	630.5	662.5	699.2	741.4	790.6	848.6	918.1
10.00	559.2	582.8	609.4	639.3	673.3	712.4	757.7	810.9	874.1
15.00	542.6	564.8	589.7	617.7	649.4	685.7	727.6	776.5	834.4
20.00	526.9	547.9	571.3	597.5	627.2	661.0	699.9	745.1	798.2
25.00	512.2	532.0	554.1	578.7	606.5	638.1	674.3	716.2	765.2
30.00	498.4	517.1	537.9	561.1	587.3	616.8	650.6	689.6	734.9
35.00	485.3	503.0	522.7	544.6	569.2	597.0	628.6	664.9	707.1
40.00	472.9	489.7	508.4	529.1	552.3	578.4	608.1	642.1	681.3
45.00	461.1	477.2	494.9	514.5	536.4	561.1	589.0	620.8	657.5
50.00	450.0	465.2	482.1	500.7	521.5	544.8	571.0	601.0	635.4
55.00	439.4	453.9	469.9	487.7	507.4	529.4	554.2	582.4	614.7
60.00	429.3	443.2	458.5	475.3	494.0	514.9	538.4	565.1	595.5

Table S4. Continued

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
BB									
0.10	597.2	622.3	650.7	683.4	721.2	765.6	818.3	882.0	960.3
1.00	593.6	618.4	646.5	678.8	716.1	759.8	811.7	874.3	951.2
5.00	578.5	602.0	628.6	659.0	694.1	735.1	783.6	841.8	912.9
10.00	560.6	582.7	607.6	635.9	668.6	706.6	751.2	804.6	869.3
15.00	543.9	564.6	588.0	614.5	644.9	680.2	721.6	770.6	829.9
20.00	528.1	547.7	569.6	594.5	623.0	655.9	694.2	739.6	794.0
25.00	513.3	531.8	552.5	575.9	602.5	633.3	669.0	711.0	761.2
30.00	499.4	516.8	536.4	558.4	583.5	612.2	645.6	684.7	731.2
35.00	486.2	502.7	521.2	542.0	565.6	592.6	623.9	660.4	703.5
40.00	473.7	489.4	506.9	526.6	548.9	574.3	603.6	637.8	678.0
45.00	461.9	476.8	493.4	512.1	533.1	557.1	584.7	616.7	654.3
50.00	450.7	464.9	480.7	498.4	518.3	541.0	567.0	597.1	632.3
55.00	440.0	453.6	468.6	485.4	504.3	525.8	550.4	578.7	611.8
60.00	429.9	442.8	457.1	473.1	491.1	511.5	534.7	561.5	592.7
PA									
0.10	538.2	564.4	594.2	628.3	667.7	713.6	767.9	832.7	911.6
1.00	535.4	561.4	590.8	624.6	663.5	708.8	762.3	826.2	903.8
5.00	523.6	548.4	576.4	608.5	645.4	688.2	738.5	798.3	870.6
10.00	509.5	533.0	559.5	589.6	624.2	664.2	710.9	766.2	832.5
15.00	496.2	518.4	543.5	571.9	604.4	641.8	685.4	736.6	797.7
20.00	483.7	504.7	528.5	555.3	585.9	621.0	661.7	709.4	765.9
25.00	471.7	491.8	514.3	539.7	568.5	601.5	639.7	684.2	736.7
30.00	460.4	479.5	500.9	524.9	552.2	583.3	619.2	660.8	709.7
35.00	449.6	467.8	488.2	511.0	536.8	566.2	600.0	639.0	684.7
40.00	439.4	456.8	476.1	497.9	522.4	550.2	582.0	618.7	661.5
45.00	429.6	446.2	464.7	485.4	508.7	535.0	565.1	599.7	639.8
50.00	420.3	436.2	453.8	473.6	495.7	520.8	549.2	581.9	619.7
55.00	411.4	426.6	443.5	462.3	483.5	507.3	534.3	565.2	600.8
60.00	402.9	417.5	433.6	451.7	471.8	494.5	520.1	549.4	583.1
MS									
0.10	477.5	501.7	528.4	558.1	591.2	628.1	669.4	716.0	768.5
1.00	475.2	499.1	525.6	555.0	587.6	624.1	664.9	710.8	762.5
5.00	465.2	488.1	513.4	541.4	572.4	607.0	645.5	688.7	737.1
10.00	453.3	475.0	498.9	525.3	554.5	586.9	622.9	662.9	707.8
15.00	442.0	462.7	485.3	510.3	537.8	568.2	601.8	639.2	680.7
20.00	431.3	451.0	472.5	496.1	522.0	550.6	582.2	617.1	655.8
25.00	421.2	439.9	460.3	482.7	507.2	534.2	563.9	596.6	632.7
30.00	411.5	429.3	448.8	470.0	493.3	518.8	546.7	577.5	611.2
35.00	402.2	419.3	437.8	458.1	480.1	504.3	530.7	559.6	591.3
40.00	393.4	409.7	427.4	446.7	467.7	490.6	515.5	542.8	572.6
45.00	385.0	400.6	417.5	435.9	455.9	477.6	501.3	527.1	555.1
50.00	377.0	391.9	408.1	425.7	444.7	465.4	487.8	512.2	538.8
55.00	369.3	383.6	399.1	415.9	434.1	453.8	475.1	498.3	523.4
60.00	361.9	375.7	390.6	406.6	424.0	442.8	463.1	485.1	508.9

Table S5. Internal Pressure, P_i (MPa), of Pure Solvents as a Function of Pressure and Temperature

P (MPa)	$T(K)$								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
MB									
0.10	434.1	439.5	442.9	444.3	443.2	439.7	433.2	423.7	410.7
1.00	434.2	439.5	442.9	444.2	443.2	439.5	433.0	423.3	410.1
5.00	434.3	439.6	443.0	444.1	442.8	438.8	431.8	421.4	407.3
10.00	434.5	439.8	443.0	443.9	442.3	437.9	430.2	419.0	403.8
15.00	434.6	439.8	442.9	443.7	441.8	436.9	428.6	416.6	400.2
20.00	434.7	439.9	442.9	443.4	441.2	435.8	427.0	414.0	396.5
25.00	434.8	439.9	442.8	443.1	440.5	434.7	425.2	411.5	392.7
30.00	434.8	439.9	442.6	442.7	439.8	433.6	423.5	408.8	388.9
35.00	434.9	439.8	442.4	442.3	439.1	432.4	421.6	406.1	385.0
40.00	434.9	439.8	442.2	441.9	438.4	431.2	419.7	403.3	381.0
45.00	434.8	439.6	442.0	441.4	437.6	429.9	417.8	400.5	377.0
50.00	434.8	439.5	441.7	440.9	436.7	428.6	415.8	397.7	372.9
55.00	434.7	439.3	441.4	440.4	435.8	427.2	413.8	394.7	368.7
60.00	434.5	439.2	441.0	439.8	434.9	425.8	411.8	391.8	364.5
EB									
0.10	400.2	404.0	406.2	406.6	405.2	401.7	396.0	388.0	377.3
1.00	400.5	404.3	406.4	406.9	405.4	401.9	396.2	388.0	377.2
5.00	401.5	405.4	407.6	408.0	406.5	402.8	396.8	388.2	376.8
10.00	402.8	406.7	409.0	409.3	407.7	403.8	397.4	388.4	376.3
15.00	404.0	408.0	410.3	410.6	408.9	404.7	398.0	388.5	375.6
20.00	405.2	409.3	411.6	411.9	410.0	405.6	398.6	388.5	374.9
25.00	406.4	410.5	412.8	413.1	411.0	406.5	399.0	388.4	374.0
30.00	407.5	411.7	414.0	414.2	412.0	407.2	399.4	388.2	373.1
35.00	408.7	412.9	415.2	415.3	413.0	407.9	399.8	388.0	372.1
40.00	409.7	414.0	416.3	416.4	413.9	408.6	400.1	387.7	371.1
45.00	410.8	415.1	417.4	417.4	414.8	409.2	400.3	387.4	369.9
50.00	411.8	416.1	418.4	418.4	415.6	409.8	400.4	387.0	368.7
55.00	412.7	417.2	419.4	419.3	416.4	410.3	400.6	386.5	367.5
60.00	413.7	418.2	420.4	420.2	417.1	410.8	400.6	386.0	366.1
PB									
0.10	386.0	390.4	393.2	394.1	393.1	389.7	384.0	375.4	363.7
1.00	386.3	390.7	393.5	394.4	393.3	390.0	384.1	375.4	363.5
5.00	387.7	392.1	394.9	395.8	394.5	390.8	384.5	375.2	362.5
10.00	389.4	393.9	396.6	397.4	395.9	391.9	385.0	374.9	361.0
15.00	391.1	395.6	398.3	399.0	397.2	392.9	385.4	374.5	359.5
20.00	392.7	397.3	400.0	400.5	398.5	393.8	385.8	374.1	358.0
25.00	394.3	398.9	401.6	402.0	399.8	394.7	386.1	373.6	356.3
30.00	395.9	400.5	403.1	403.4	401.0	395.5	386.3	373.0	354.5
35.00	397.4	402.1	404.6	404.8	402.1	396.2	386.5	372.3	352.7
40.00	398.9	403.6	406.1	406.1	403.2	396.9	386.6	371.6	350.8
45.00	400.3	405.1	407.5	407.4	404.3	397.6	386.7	370.8	348.8
50.00	401.8	406.5	408.9	408.7	405.3	398.2	386.7	369.9	346.8
55.00	403.2	407.9	410.3	409.9	406.2	398.7	386.6	369.0	344.7
60.00	404.5	409.3	411.6	411.1	407.1	399.2	386.5	368.1	342.5

Table S5. Continued

P (MPa)	T(K)								
	278.15	288.15	298.15	308.15	318.15	328.15	338.15	348.15	358.15
BB									
0.10	375.4	380.0	382.9	383.8	382.6	378.9	372.4	362.8	349.7
1.00	375.7	380.3	383.2	384.1	382.8	379.0	372.4	362.6	349.2
5.00	377.3	381.8	384.6	385.4	383.8	379.6	372.3	361.6	347.0
10.00	379.1	383.7	386.4	386.9	385.0	380.2	372.2	360.4	344.2
15.00	380.9	385.5	388.1	388.4	386.1	380.8	372.0	359.0	341.3
20.00	382.7	387.3	389.7	389.8	387.2	381.3	371.7	357.6	338.3
25.00	384.5	389.0	391.4	391.2	388.2	381.8	371.3	356.1	335.2
30.00	386.2	390.7	392.9	392.6	389.2	382.2	370.9	354.6	332.0
35.00	387.9	392.3	394.5	393.9	390.1	382.5	370.4	352.9	328.8
40.00	389.5	394.0	396.0	395.2	391.0	382.8	369.9	351.3	325.5
45.00	391.2	395.6	397.4	396.4	391.8	383.1	369.3	349.5	322.1
50.00	392.7	397.1	398.9	397.6	392.6	383.3	368.7	347.7	318.7
55.00	394.3	398.6	400.3	398.7	393.3	383.4	368.0	345.8	315.2
60.00	395.8	400.1	401.6	399.8	394.1	383.6	367.3	343.9	311.7
PA									
0.10	447.8	452.5	455.0	455.3	453.0	447.9	439.7	428.2	412.9
1.00	448.1	452.7	455.3	455.5	453.2	448.0	439.7	428.0	412.5
5.00	449.2	453.8	456.3	456.4	453.8	448.3	439.6	427.2	410.6
10.00	450.5	455.1	457.6	457.5	454.7	448.7	439.3	426.0	408.3
15.00	451.8	456.4	458.8	458.5	455.4	449.1	439.0	424.8	405.8
20.00	453.1	457.7	459.9	459.5	456.1	449.3	438.6	423.5	403.2
25.00	454.3	458.9	461.1	460.5	456.8	449.5	438.2	422.2	400.6
30.00	455.5	460.1	462.2	461.4	457.4	449.7	437.7	420.7	397.8
35.00	456.7	461.3	463.2	462.3	458.0	449.8	437.1	419.2	395.0
40.00	457.8	462.4	464.3	463.1	458.5	449.8	436.5	417.7	392.2
45.00	458.9	463.4	465.2	463.9	458.9	449.8	435.8	416.0	389.2
50.00	460.0	464.5	466.2	464.6	459.4	449.8	435.1	414.4	386.2
55.00	461.1	465.5	467.1	465.3	459.8	449.7	434.3	412.6	383.1
60.00	462.1	466.5	468.0	466.0	460.1	449.6	433.5	410.8	380.0
MS									
0.10	450.3	453.8	455.9	456.4	455.2	452.5	448.1	442.1	434.5
1.00	450.4	454.0	456.0	456.5	455.4	452.6	448.3	442.3	434.6
5.00	450.8	454.4	456.6	457.1	456.0	453.3	449.0	443.0	435.3
10.00	451.2	455.0	457.2	457.8	456.8	454.2	449.8	443.8	436.1
15.00	451.6	455.5	457.8	458.5	457.6	454.9	450.6	444.6	436.8
20.00	452.0	456.0	458.4	459.2	458.3	455.7	451.3	445.3	437.4
25.00	452.4	456.4	458.9	459.8	458.9	456.3	452.0	445.9	438.0
30.00	452.7	456.9	459.4	460.3	459.5	457.0	452.6	446.5	438.5
35.00	453.0	457.3	459.9	460.9	460.1	457.5	453.2	447.0	439.0
40.00	453.3	457.6	460.3	461.3	460.6	458.1	453.7	447.5	439.4
45.00	453.5	458.0	460.7	461.8	461.1	458.6	454.2	447.9	439.7
50.00	453.8	458.3	461.1	462.2	461.6	459.0	454.6	448.3	440.0
55.00	454.0	458.6	461.5	462.6	462.0	459.4	455.0	448.6	440.2
60.00	454.2	458.8	461.8	463.0	462.4	459.8	455.3	448.9	440.4

Table S6. EOS parameters, absolute average deviations, AAD, and deviations (calculated - experimental) in critical temperature, ΔT_C , and pressure, ΔP_C , obtained from the simultaneous correlation of saturation pressure and saturated liquid density obtained from the reported literature references in the showed reduced temperature ranges, T_r . For MS results with different association schemes¹⁵ are reported. TRIDEN means data calculated under P/T saturation conditions using the TRIDEN parameters reported in Table S2 (Supporting Information). Superindices in ΔT_C and ΔP_C columns show the literature reference from which experimental critical properties were obtained

	SAFT	m	v_{00} / mL mol ⁻¹	u_0 / k / K	ϵ^{AB} / k / K	K^{AB}	AAD	ΔT_C / K	ΔP_C / MPa	T_r range	reference for saturation	saturated pressure	liquid density	reference for saturation	saturated pressure	liquid density
MB	5.657	11.300	262.64	—	—	3.42	2.35	31.59 ³⁸	0.36 ³⁸	0.46-0.75	38	38	38	38	38	38
EB	7.257	9.713	234.56	—	—	4.72	3.02	12.73 ³⁸	0.04 ³⁸	0.46-0.74	38	38	38	38	38	38
PB	5.524	15.468	278.80	—	—	3.41	1.06	5.02 ^a	0.40 ^a	0.42-0.66	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
BB	6.264	14.977	271.12	—	—	6.61	1.93	64.05 ³⁹	0.47 ³⁹	0.39-0.72	39	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
PA	6.915	9.076	234.70	—	—	4.31	1.94	22.14 ⁴⁰	0.38 ⁴⁰	0.48-0.74	40	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
MS - 2B	4.759	14.541	296.31	1686.14	0.020407	0.45	6.65	67.11 ¹⁸	0.51 ¹⁸	0.46-0.72	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
MS - 3B	5.100	13.379	286.39	1485.06	0.012728	0.36	6.80	62.22 ¹⁸	0.43 ¹⁸	0.46-0.72	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
PC-SAFT	m	$\sigma / \text{\AA}$	$\epsilon / k / \text{K}$	$\epsilon^{AB} / k / \text{K}$	K^{AB}	AAD	AAD	ΔT_C / K	ΔP_C / MPa	T_r range	reference for saturation	saturated pressure	liquid density	reference for saturation	saturated pressure	liquid density
MB	3.657	3.6412	304.91	—	—	2.79	0.49	17.99 ³⁸	0.56 ³⁸	0.46-0.75	38	38	38	38	38	38
EB	4.636	3.5045	274.08	—	—	5.39	0.15	0.17 ³⁸	0.36 ³⁸	0.46-0.74	38	38	38	38	38	38
PB	3.587	4.0173	322.70	—	—	2.75	1.25	-19.83 ^a	0.59 ^a	0.42-0.66	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
BB	4.096	3.9644	312.50	—	—	5.37	1.01	47.85 ³⁹	0.74 ³⁹	0.39-0.72	39	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
PA	4.446	3.4136	273.38	—	—	3.46	0.89	9.32 ⁴⁰	0.70 ⁴⁰	0.48-0.74	40	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
MS - 2B	3.034	3.9521	340.12	1577.87	0.024986	1.40	5.17	49.59 ¹⁸	0.68 ¹⁸	0.46-0.72	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN
MS - 3B	2.437	4.2909	372.06	1720.31	0.014071	1.73	5.03	57.00 ¹⁸	0.77 ¹⁸	0.46-0.72	18	TRIDEN	TRIDEN	TRIDEN	TRIDEN	TRIDEN

^a Experimental properties calculated according to Joback's method^[4]

Table S7. Aromatic esters parameters used in the IEF-PCM calculations. ε = dielectric constant, ε_∞ ($= n_D^2$) dielectric constant at infinite frequency, R = solvent radius and d = solvent particle density.

	MB	EB	PB	BB	PA	MS
ε^a	6.6	6.0	5.8	5.5	2.4	8.8
ε_∞^b	2.29	2.26	2.25	2.24	2.25	2.36
$R / \text{\AA}^c$	5.93	6.21	6.45	6.66	5.95	5.98
$d / \text{\AA}^{-3}c$	0.00478963	0.00417463	0.00372668	0.00338101	0.00473611	0.00465729

^a Ref. 56; ^b From refractive indices reported in Ref. 11a, except MS for which n_D was obtained from Ref. 56; ^c From density data at 298.15 K and 0.1 MPa reported in Table S1.