TABLE V: Numerical data for the saturated liquid and vapor densities and the saturated vapor pressures obtained from the Gibbs ensemble Monte Carlo simulations for ethers and glycols. Subscripts indicate uncertainty in the final digit.

molecule	T [K]	ρ_{liq} [g cm^{-3}]	ρ_{vap} [g cm^{-3}]	p [kPa]
dimethyl ether	273.35	0.00669_6	0.6966_6	308_3
	303	0.0179_{10}	0.6486_{11}	839_{39}
	329.2	0.0343_8	0.6037_7	1583_{24}
	353.3	0.0551_{36}	0.5490_{17}	2493_{96}
	369.67	0.0730_{39}	0.4969_{40}	3252_{92}
ethyl methyl ether	273.15	0.00288_5	0.7191_9	105_2
	323.15	0.0138_7	0.6520_{10}	543_{24}
	351.45	0.0253_9	0.6061_7	1025_{30}
	367.65	0.0386_{20}	0.5795_{11}	1530_{56}
	392.45	0.0683_{27}	0.5248_{18}	2472_{46}
	403.15	0.0806_{31}	0.4986_{29}	2867_{50}
diethyl ether	303.15	0.00378_7	0.7006_9	123_2
	343.15	0.0116_9	0.6498_{13}	401_{27}
	393.15	0.0352_{10}	0.5728_{13}	1202_{23}
	423.15	0.0678_{46}	0.5128_{30}	2134_{70}
methyl t-butyl ether	298.15	0.00178_8	0.7462_{14}	49.0_{19}
	323.15	0.00407_6	0.7189_4	119_2
	373.15	0.0165_4	0.6572_9	511_{11}
	443.15	0.0606_{22}	0.5396_{25}	1820_{36}
diisopropyl ether	300	0.00144_1	0.7377_{11}	34.5_3
	350	0.00696_{31}	0.6770_6	184_8
	400	0.0228_8	0.6077_{22}	622_{19}
	425	0.0401_{27}	0.5669_{22}	1069_{52}
dipropyl ether	325	0.00157_{10}	0.7110_3	40.6_{26}
	375	0.00741_{14}	0.6557_5	209_4
	425	0.0214_8	0.5910_{10}	619_{18}
	475	0.0673_{28}	0.5092_{21}	1690_{36}
1,2-dimethoxyethane	325	0.00096_3	0.8442_8	28.4_7
	375	0.00565_{13}	0.7823_{15}	185_4
	425	0.0193_9	0.7118_{15}	648_{25}
	475	0.0504_{22}	0.6222_{20}	1629_{44}

1,2-ethanediol	450	0.00095_{4}	0.9837_{14}	55.3_{27}
	500	0.00432_{16}	0.9318_{16}	272_{11}
	550	0.00999_{63}	0.8545_{31}	656_{36}
	600	0.0297_{5}	0.7845_{44}	1903_{32}
	650	0.0624_{39}	0.6696_{91}	3899_{162}
1,3-propanediol	450	0.00051_{3}	0.9362_{14}	25.1_{13}
	500	0.00316_{8}	0.8846_{29}	166_{4}
	550	0.00904_{54}	0.8254_{21}	499_{26}
	600	0.0240_{17}	0.7583_{24}	1311_{77}
	650	0.0570_{19}	0.6664_{19}	2883_{74}
2-methoxyethan-1-ol	347.7	0.00050_{2}	0.9171_{12}	18.5_{6}
	397.7	0.00365_{9}	0.8643_{11}	150_{3}
	450	0.0127_{6}	0.7873_{17}	555_{20}
	500	0.0345_{9}	0.7020_{27}	1514_{37}
	550	0.0988_{38}	0.5920_{41}	3561_{76}

TABLE VI: Numerical data for the saturated liquid and vapor densities and the saturated vapor pressures obtained from the grand canonical Monte Carlo simulations for aldehydes and ketones.

molecule	T [K]	ρ_{liq} [g cm^{-3}]	ρ_{vap} [g cm^{-3}]	p [kPa]
acetaldehyde	260	0.00055	0.8251	18.5
	300	0.00267	0.7754	135
	340	0.00881	0.7200	495
	380	0.02336	0.6556	1324
	420	0.05741	0.5691	2926
	440	0.09429	0.5027	4146
pentanal	300	0.00021	0.8145	6.07
	340	0.00109	0.7762	35.7
	380	0.00369	0.7320	133
	420	0.00961	0.6872	364
	460	0.02189	0.6367	824
	500	0.04619	0.5729	1637
	540	0.09955	0.4767	2948
octanal	360	0.00047	0.7654	10.7
	400	0.00179	0.7268	44.7
	440	0.00514	0.6916	137
	480	0.01234	0.6487	339
	520	0.02612	0.5988	714
	560	0.05264	0.5373	1339
	600	0.11719	0.4541	2332
acetone	300	0.00110	0.7733	42.3
	340	0.00436	0.7290	182
	380	0.01232	0.6811	556
	420	0.02822	0.6262	1317
	460	0.05974	0.5561	2644
	500	0.13435	0.4359	4770
2-pentanone	300	0.00026	0.7944	7.44
	340	0.00123	0.7573	39.7
	380	0.00400	0.7183	140
	420	0.01021	0.6741	378
	460	0.02234	0.6245	836
	500	0.04535	0.5675	1621
	540	0.09534	0.4840	2864

2-octanone	360	0.00033	0.7662	4.43
	400	0.00133	0.7310	29.7
	440	0.00398	0.6963	103
	480	0.00927	0.6548	266
	520	0.01881	0.6119	560
	560	0.03666	0.5595	1047
	600	0.07161	0.4886	1806
	620	0.10181	0.4352	2314

TABLE VII: Numerical data for the liquid and vapor phase compositions obtained from the constant-pressure Gibbs ensemble Monte Carlo simulations for the binary mixture of diethyl ether and ethanol at $T = 283.15$ K. Subscripts indicate uncertainty in the final digit.

p [kPa]	x_{DEE}	y_{DEE}
2.8	0	0
10	0.050_3	0.721_{13}
15	0.103_3	0.837_5
25	0.229_{10}	0.910_7
30	0.327_8	0.930_6
35	0.444_8	0.942_7
45	0.656_3	0.963_1
50	0.782_4	0.971_2
52.3	1	1

TABLE VIII: Numerical data for the pressure and liquid and vapor phase compositions obtained from the grand canonical Monte Carlo simulations for the binary mixture of acetone and hexane at $T = 328.15$ K.

p [kPa]	x_{acetone}	y_{acetone}
150.90	0.999	0.999
152.29	0.982	0.973
153.62	0.968	0.950
156.03	0.938	0.909
157.71	0.911	0.878
159.59	0.867	0.836
161.25	0.799	0.779
161.56	0.683	0.699
156.15	0.463	0.574
154.84	0.434	0.557
153.33	0.404	0.538
151.57	0.373	0.518
149.54	0.340	0.495
147.19	0.307	0.471
144.49	0.273	0.444
141.36	0.238	0.413
137.80	0.204	0.379
133.71	0.169	0.340
129.05	0.134	0.294
123.71	0.100	0.241
117.60	0.066	0.178
110.53	0.032	0.100
108.99	0.026	0.082
107.40	0.019	0.063
105.77	0.013	0.044
104.06	0.006	0.023
102.30	0.000	0.001