Supporting information

Effects of temperature and solvent properties on liquid-solid phase equilibrium of γ-pyrazinamide

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Table S1 Thermodynamic parameters for γ-PZA in thirteen solvents using NRTL model (p=0.1Mpa)[a].

Solvent	*T/K*	$\Delta_{mix}G/J\cdot mol^{-1}$	$\Delta_{mix}H/J\cdot mol^{-1}$	$\Delta_{mix}S/J\cdot K^{-1}mol^{-1}$
Methanol	278.15	-26.893	0.134	0.097
	283.15	-35.987	0.168	0.128
	288.15	-42.964	0.190	0.150
	293.15	-50.844	0.220	0.174
	298.15	-58.127	0.252	0.196
	303.15	-68.735	0.309	0.228
	308.15	-76.510	0.366	0.249
	313.15	-84.829	0.441	0.272
	318.15	-101.723	0.586	0.322
Ethonal	278.15	-13.452	4.312	0.064
	283.15	-18.428	6.119	0.087
	288.15	-23.914	8.162	0.111
	293.15	-29.587	10.296	0.136
	298.15	-35.377	12.478	0.161

	303.15	-43.552	15.708	0.195
	308.15	-52.193	19.159	0.232
	313.15	-63.464	23.847	0.279
	318.15	-75.787	29.069	0.330
1-Propanol	278.15	-10.461	3.414	0.050
	283.15	-16.083	5.553	0.076
	288.15	-19.381	6.768	0.091
	293.15	-25.799	9.316	0.120
	298.15	-32.319	11.938	0.148
	303.15	-36.912	13.684	0.167
	308.15	-47.946	18.378	0.215
	313.15	-59.749	23.495	0.266
	318.15	-71.715	28.708	0.316
2-Propanol	278.15	-10.288	3.576	0.050
	283.15	-12.621	4.442	0.060
	288.15	-18.019	6.632	0.086
	293.15	-23.012	8.680	0.108
	298.15	-29.347	11.363	0.137
	303.15	-35.461	13.950	0.163
	308.15	-43.164	17.300	0.196
	313.15	-53.065	21.744	0.239
	318.15	-66.771	28.156	0.298
1-Butanol	278.15	-8.948	2.897	0.043
	283.15	-13.232	4.503	0.063
	288.15	-18.430	6.539	0.087
	293.15	-21.317	7.610	0.099
	298.15	-26.825	9.811	0.123
	303.15	-34.653	13.071	0.157
	308.15	-43.143	16.670	0.194
	313.15	-55.750	22.254	0.249

	318.15	-72.642	30.010	0.323
n-Propyl acetate	278.15	-23.122	0.094	0.083
	283.15	-30.734	0.113	0.109
	288.15	-33.946	0.115	0.118
	293.15	-39.694	0.131	0.136
	298.15	-45.655	0.153	0.154
	303.15	-53.964	0.193	0.179
	308.15	-62.889	0.248	0.205
	313.15	-70.443	0.316	0.226
	318.15	-81.199	0.420	0.257
Methyl acetate	278.15	-0.257	0.249	0.093
	283.15	-0.335	0.305	0.119
	288.15	-0.445	0.383	0.156
	293.15	-0.506	0.406	0.174
	298.15	-0.583	0.443	0.197
	303.15	-0.726	0.533	0.241
	308.15	-0.790	0.564	0.258
	313.15	-0.891	0.631	0.287
	318.15	-1.094	0.781	0.346
Ethyl acetate	278.15	-25.302	0.138	0.091
	283.15	-32.604	0.169	0.116
	288.15	-36.033	0.180	0.126
	293.15	-41.079	0.204	0.141
	298.15	-48.376	0.247	0.163
	303.15	-55.850	0.301	0.185
	308.15	-69.944	0.409	0.228
	313.15	-77.915	0.501	0.250
	318.15	-88.518	0.636	0.280
2-Butanol	278.15	-9.533	3.407	0.047

	283.15	-12.469	4.569	0.060
	288.15	-16.060	6.028	0.077
	293.15	-20.540	7.901	0.097
	298.15	-26.255	10.368	0.123
	303.15	-33.629	13.664	0.156
	308.15	-41.604	17.286	0.191
	313.15	-49.320	20.773	0.224
	318.15	-63.108	27.453	0.285
1.4-Dioxane	288.15	-0.715	8.765	0.278
	293.15	-0.894	11.237	0.343
	298.15	-1.118	14.419	0.423
	303.15	-1.326	17.380	0.495
	308.15	-1.602	21.447	0.590
	313.15	-1.817	24.521	0.659
	318.15	-2.151	29.575	0.769
Water	278.15	-10.020	3.478	0.049
	283.15	-14.806	5.394	0.071
	288.15	-19.648	7.382	0.094
	293.15	-23.143	8.759	0.109
	298.15	-29.305	11.367	0.136
	303.15	-34.588	13.555	0.159
	308.15	-44.012	17.757	0.200
	313.15	-53.534	22.038	0.241
	318.15	-64.893	27.272	0.290
Acetone	278.15	-34.018	0.041	0.122
	283.15	-41.602	0.037	0.147
	288.15	-48.665	0.035	0.169
	293.15	-57.137	0.037	0.195
	298.15	-67.035	0.047	0.225

	303.15	-77.540	0.068	0.256
	308.15	-90.342	0.104	0.294
	313.15	-103.316	0.162	0.330
	318.15	-117.097	0.246	0.369
Acetonitrile	278.15	-17.031	0.120	0.062
	283.15	-23.790	0.152	0.085
	288.15	-26.584	0.155	0.093
	293.15	-32.655	0.171	0.112
	298.15	-38.106	0.188	0.128
	303.15	-46.768	0.225	0.155
	308.15	-53.262	0.257	0.174
	313.15	-60.714	0.306	0.195
	318.15	-69.172	0.375	0.219

a. The expanded uncertainties are $U(\Delta_{mix}G) = 0.060\Delta_{mix}G$, $U(\Delta_{mix}H) = 0.055\Delta_{mix}H$, $U(\Delta_{mix}S) = 0.060\Delta_{mix}S$ (0.95 level of confidence).