

**Dataset 1.** Dataset for building the machine learning model (Training + Testing)

Experiment label	Sample label	w%	Solvent Name	Boiling Point /°C	Melting point /°C	Dielectric constant	Dipole moment /( $10^{-30}$ C · m)	Viscosity /( $\text{mPa} \cdot \text{s}$ )	Surface tension /( $\text{mN} \cdot \text{m}^{-1}$ )	Heat of evaporation /( $\text{kJ} \cdot \text{mol}^{-1}$ )	Heat capacity /( $\text{kJ} \cdot (\text{kg} \cdot \text{K})^{-1}$ )	Density /( $\text{g} \cdot \text{ml}^{-1}$ )	Soaking time /minutes	Volatilization temperature /°C	Volatilization time /h	Current Density /( $\text{mA} \cdot \text{cm}^{-2}$ )	CE /%	VE /%	EE /%
1	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	94.70	92.29	87.41
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	95.86	91.98	88.18
2	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	95.40	91.77	87.55
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	95.69	91.56	87.62
3	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	96.66	92.15	89.07
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	96.41	92.41	89.09
4	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	1	80	97.35	91.15	88.74
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	1	80	96.88	92.12	89.25
5	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	2	80	97.06	91.33	88.64
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	2	80	97.61	90.98	88.81
6	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	80	1	80	96.85	91.12	88.25
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	80	1	80	96.62	91.77	88.67
7	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	120	0.5	80	97.29	91.27	88.80
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	120	0.5	80	97.07	92.70	89.98
8	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	2	80	96.50	90.61	87.43
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	2	80	95.22	90.71	86.38
9	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	12	80	97.48	90.49	88.22
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	12	80	98.12	91.17	89.46
10	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	24	80	97.83	91.15	89.16
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	24	80	97.17	91.64	89.05
11	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	50	1	80	97.62	90.80	88.64
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	50	1	80	97.79	89.69	87.71
12	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	50	2	80	98.48	89.43	88.07
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	50	2	80	98.90	88.79	87.81
13	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	80	0.5	80	95.47	91.43	87.29
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	80	0.5	80	97.43	90.33	88.01
14	sample 1	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	80	1	80	98.95	89.04	88.10
	sample 2	13	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	80	1	80	98.51	89.44	88.10
15	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	5	50	2	80	98.00	90.90	89.08
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	5	50	2	80	97.88	91.89	89.94
16	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	10	50	2	80	95.88	91.78	88.00
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	10	50	2	80	95.63	92.09	88.07
17	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	20	50	2	80	96.09	91.55	87.97
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	20	50	2	80	95.20	92.33	87.90
18	sample 1	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	2	80	96.22	92.29	88.80
	sample 2	13	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	50	2	80	96.68	91.33	88.30
19	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	40	96.53	95.89	92.57
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	40	97.39	95.97	93.47
20	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	60	97.73	93.83	91.70
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	60	98.31	94.04	92.45
21	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	98.25	91.84	90.23
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	98.60	92.17	90.88
22	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	100	98.68	89.92	88.74

Data lable		w%	Solvent Name	Boiling Point /°C	Melting point /°C	Dielectric constant	Dipole moment /( $10^{-30}$ C · m)	Viscosity /( $\text{mPa s}$ )	Surface tension /( $\text{mN m}^{-1}$ )	Heat of evaporation /( $\text{kJ mol}^{-1}$ )	Heat capacity /( $\text{kJ}/(\text{kg} \cdot \text{K})$ )	Density /( $\text{g ml}^{-1}$ )	Soaking time /minutes	Volatilization temperature /°C	Volatilization time /h	Current Density /( $\text{mA cm}^{-2}$ )	CE /%	VE /%	EE /%
22	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	100	98.87	90.37	89.34
23	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	120	98.88	88.42	87.43
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	120	99.04	88.63	87.78
24	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	140	99.06	86.72	85.90
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	140	99.27	87.06	86.43
25	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	160	98.81	84.86	83.86
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	160	99.14	85.48	84.74
26	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	200	99.19	81.44	80.78
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	200	99.29	82.51	81.93
27	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	1	80	97.74	90.96	88.90
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	1	80	98.27	90.68	89.11
28	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	97.26	92.15	89.62
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	98.06	91.68	89.91
29	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	97.50	90.99	88.71
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	96.11	91.12	87.58
30	sample 1	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	98.73	91.74	90.57
	sample 2	15	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	98.28	91.39	89.82
31	sample 1	15	hexane	68.7	-95.3	1.89	0.27	0.31	17.90	33.12	2.28	0.6590	30	25	12	80	96.14	89.56	86.10
	sample 2	15	hexane	68.7	-95.3	1.89	0.27	0.31	17.90	33.12	2.28	0.6590	30	25	12	80	96.80	90.61	87.70
32	sample 1	15	hexane	68.7	-95.3	1.89	0.27	0.31	17.90	33.12	2.28	0.6590	30	25	24	80	98.20	89.41	87.80
	sample 2	15	hexane	68.7	-95.3	1.89	0.27	0.31	17.90	33.12	2.28	0.6590	30	25	24	80	98.54	88.99	87.69
33	sample 1	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	0.5	80	97.09	92.27	89.59
	sample 2	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	0.5	80	98.60	91.75	90.47
34	sample 1	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	1	80	98.83	91.57	90.49
	sample 2	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	1	80	98.35	90.50	89.01
35	sample 1	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	2	80	97.76	91.69	89.64
	sample 2	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	2	80	98.98	90.41	89.49
36	sample 1	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	12	80	98.03	91.39	89.59
	sample 2	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	12	80	97.27	91.02	88.53
37	sample 1	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	24	80	98.29	91.78	90.21
	sample 2	15	ethanol	78.3	-114.5	25.7	5.60	1.06	22.10	38.59	2.42	0.7893	30	25	24	80	97.91	90.69	88.80
38	sample 1	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	2	80	95.60	90.72	86.73
	sample 2	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	2	80	96.83	90.19	87.34
39	sample 1	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	12	80	98.90	90.31	89.31
	sample 2	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	12	80	98.59	90.48	89.21
40	sample 1	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	24	80	98.64	90.25	89.02
	sample 2	15	water	100.0	0.0	78.5	6.18	1.01	72.75	40.67	4.19	1.0000	30	25	24	80	98.64	90.25	89.02
41	sample 1	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	0.5	80	94.55	91.05	86.09
	sample 2	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	0.5	80	94.68	90.24	85.44
42	sample 1	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	1	80	98.95	89.74	88.80
	sample 2	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	1	80	99.18	88.59	87.87
43	sample 1	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	2	80	98.53	90.13	88.81
	sample 2	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	2	80	99.00	88.42	87.54
44	sample 1	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	12	80	98.53	90.19	88.87

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44	sample 2	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	12	80	99.08	89.46	88.64
45	sample 1	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	24	80	99.17	89.42	88.68
	sample 2	15	acetone	56.1	-94.7	20.7	8.97	0.32	23.70	29.11	1.28	0.7906	30	25	24	80	98.95	88.57	87.64
46	sample 1	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	0.5	80	94.30	92.43	87.16
	sample 2	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	0.5	80	95.88	92.06	88.27
47	sample 1	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	94.69	91.86	86.99
	sample 2	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	2	80	94.65	92.25	87.31
48	sample 1	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	96.53	90.81	87.67
	sample 2	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	12	80	98.40	91.70	90.23
49	sample 1	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	98.28	91.60	90.03
	sample 2	17	IPA	82.4	-89.5	18.3	5.60	2.43	21.70	40.06	2.55	0.7863	30	25	24	80	97.55	91.44	89.20