

Property	ML	TRAIN			TEST		
		R2	RMSE	MAE	R2	RMSE	MAE
CO2 capacity	CUBIST	0.98	0.0291	0.0107	0.81	0.1081	0.0689
	GBM	0.98	0.0303	0.0134	0.86	0.0915	0.0574
	RF	0.82	0.0994	0.0772	0.63	0.1588	0.1281
Electrical conductivity	CUBIST	0.99	0.0363	0.0071	0.75	0.1597	0.1036
	GBM	0.98	0.0464	0.0118	0.79	0.1456	0.0990
	RF	0.96	0.0676	0.0213	0.73	0.1658	0.1120
Density	CUBIST	0.99	14.8745	0.2817	0.75	94.4408	58.8625
	GBM	0.99	12.2322	2.6455	0.93	49.1054	28.3450
	RF	0.99	19.8324	8.9915	0.89	61.1986	39.1206
T _g	CUBIST	0.62	21.3054	2.2186	0.62	18.6955	12.3427
	GBM	0.59	22.5628	4.1693	0.59	19.4345	13.3378
	RF	0.60	21.9156	5.9943	0.55	19.4437	13.1731
T _m	CUBIST	0.67	44.4787	12.1433	0.65	45.9665	33.4230
	GBM	0.66	45.2619	13.3301	0.67	44.9742	33.2290
	RF	0.67	44.3158	14.5775	0.66	45.5516	33.4486
Heat Capacity	CUBIST	1.00	0.0497	0.0063	0.90	0.2855	0.1772
	GBM	1.00	0.0423	0.0124	0.91	0.2766	0.1931
	RF	1.00	0.0501	0.0067	0.89	0.3051	0.2089
Refractive Index	CUBIST	0.97	0.0064	0.0004	0.84	0.0164	0.0108
	GBM	0.98	0.0057	0.0012	0.82	0.0172	0.0111
	RF	0.97	0.0066	0.0022	0.81	0.0179	0.0114
T _d	CUBIST	0.77	38.3210	6.2270	0.76	39.3396	27.7529
	GBM	0.74	41.0204	16.9702	0.79	36.3565	27.1693
	RF	0.77	38.7145	12.0973	0.80	35.4431	25.2845
Viscosity	CUBIST	0.95	0.1567	0.0208	0.72	0.3816	0.2601
	GBM	0.94	0.1739	0.0577	0.76	0.3519	0.2354
	RF	0.91	0.2158	0.0717	0.66	0.4181	0.2816
Cytotoxicity	CUBIST	0.80	0.5109	0.2122	0.79	0.4733	0.3508
	GBM	0.79	0.5148	0.1215	0.77	0.5055	0.3845
	RF	0.80	0.4896	0.1532	0.78	0.4931	0.3607
Surface Tension	CUBIST	0.97	0.0014	0.0002	0.77	0.0043	0.0027
	GBM	0.97	0.0014	0.0003	0.79	0.0041	0.0027
	RF	0.97	0.0016	0.0004	0.74	0.0045	0.0031
Thermal conductivity	CUBIST	0.95	0.0054	0.0014	0.85	0.0101	0.0060
	GBM	0.95	0.0055	0.0015	0.89	0.0089	0.0056
	RF	0.94	0.0059	0.0017	0.87	0.0100	0.0073

Table 1: Summary of the ML performances for 12 different IL properties.