Supporting Information – Metrics

A consistent set of thermophysical properties of methane curated with machine learning

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Introduction

The present document is divided into three sections. The sections first present the performance metrics of the best Machine Learning (ML) models for predicting the various thermophysical properties and then the performance metrics for all the ML models used for each property. They are subdivided by the thermodynamic phase of matter: liquid (S1. Liquid Phase), vapor (S2. Vapor Phase), and supercritical (S3. Supercritical Phase).

S1. Liquid Phase

S1.1 Best metrics

On Table S1, the units of MAE and RMSE are reported in the same units as the target property, while MSE carries squared units. For instance, when predicting density ($kg \cdot m^{-3}$) or sound speed ($m \cdot s^{-1}$), MAE and RMSE are expressed in $kg \cdot m^{-3}$ and $m \cdot s^{-1}$, respectively, while MSE carries squared units, such as $(kg \cdot m^{-3})^2$ or $(m \cdot s^{-1})^2$. The MAPE, in contrast, is unitless and expressed as a percentage. The R^2 metric is also unitless

Tables odd-numbered from Table S3 to Table S15 presents all the ML performance metrics for predicting the corresponding investigated property in liquid phase. Data in red represents the best model for each property.

Table S1: ML performance metrics for the best-performing models for predicting various thermophysical properties in the liquid phase: Density ($kg \cdot m^{-3}$), Volume ($m^3 \cdot kg^{-1}$), Enthalpy ($kJ \cdot mol^{-1}$), $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$), $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$), Sound Speed ($m \cdot s^{-1}$), and Viscosity (µPa·s). The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in the respective property units are presented.

Cp – Random Forest – CV =LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	2 %	5.038	2912.242	53.965	0.140
Exp x NIST	1 %	4.215	2820.264	53.106	0.167
NIST x Model	1 %	1.204	20.053	4.478	0.927
Cv – ExtraTrees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	2 %	0.471	1.927	1.388	0.598
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.365	0.225	0.474	0.9
Sound Speed – ExtraTrees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	8.%	35.365	8888.332	94.278	0.947
Exp x NIST	6.%	25.674	11763.196	108.458	0.93
NIST x Model	7.%	34.951	8154.814	90.304	0.95
Density – Gradient Boosting – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	6 %	7.268	773.878	27.819	0.794
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	1 %	4.508	124.334	11.151	0.961
Volume – Decision Tree – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	3 %	0	0	0.002	0.071
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	2 %	0	0	0	0.772
Enthalpy – Gradient Boosting – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	1532755325052460 %	0.16	0.131	0.362	0.955
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	226 %	0.521	0.291	0.54	0.902
Viscosity – Extra Trees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	39 %	25.737	1318.966	36.318	0.682
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	21 %	19.165	700.412	26.465	0.762

S1.2 Isobaric heat capacity (Cp)

Table S2: Evaluation of multiple ML models for $\boldsymbol{Cp}$ in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
BaggingRegressor	0.98	0.98	2.16
RandomForestRegressor	0.97	0.97	2.43
GradientBoostingRegressor	0.96	0.96	2.72
KNeighborsRegressor	0.96	0.96	2.88
ExtraTreesRegressor	0.95	0.96	3.01
XGBRegressor	0.95	0.96	3.03
DecisionTreeRegressor	0.91	0.91	4.22
AdaBoostRegressor	0.81	0.82	6.07
PassiveAggressiveRegressor	0.69	0.71	7.79
NuSVR	0.65	0.67	8.28
SVR	0.65	0.67	8.34
GammaRegressor	0.61	0.63	8.74
ElasticNet	0.56	0.58	9.39
TweedieRegressor	0.54	0.57	9.49
HuberRegressor	0.54	0.57	9.50
HistGradientBoostingRegressor	0.44	0.47	10.56
LGBMRegressor	0.44	0.47	10.57
OrthogonalMatchingPursuit	0.43	0.46	10.64
ExtraTreeRegressor	0.37	0.40	11.17
LinearSVR	0.37	0.40	11.21
ElasticNetCV	0.36	0.39	11.29
RANSACRegressor	0.33	0.36	11.55
BayesianRidge	0.29	0.33	11.84
PoissonRegressor	0.25	0.29	12.21
Lasso	0.22	0.26	12.46
LassoLars	0.22	0.26	12.46
RidgeCV	0.20	0.24	12.61
LassoCV	0.11	0.15	13.29
Ridge	0.07	0.12	13.57
TransformedTargetRegressor	0.05	0.10	13.69
LinearRegression	0.05	0.10	13.69
LarsCV	0.05	0.10	13.69
OrthogonalMatchingPursuitCV	0.05	0.10	13.69
LassoLarsIC	0.05	0.10	13.69
LassoLarsCV	0.05	0.10	13.69
Lars	0.05	0.10	13.69

SGDRegressor	0.03	0.09	13.82
DummyRegressor	-0.18	-0.11	15.26
MLPRegressor	-17.71	-16.73	60.87
KernelRidge	-22.66	-21.42	68.45
GaussianProcessRegressor	-85.22	-80.68	130.66

Table S3: ML performance metrics for predicting $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20 %	17.15	3255	57.05	0.039
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	20 %	13.38	268.8	16.39	0.02
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	12.09	3149	56.11	0.07
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	11 %	8.259	158.9	12.6	0.421
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20 %	17.28	3257	57.07	0.038
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	20 %	13.51	274.2	16.56	0
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	12.16	3147	56.1	0.071
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	12 %	8.336	159.9	12.65	0.417
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	16 %	14.85	3185	56.43	0.06
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	16 %	11.04	192.6	13.88	0.298
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	15.07	3172	56.32	0.064
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	17 %	11.27	189.1	13.75	0.311
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	14.95	3185	56.44	0.06
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	16 %	11.14	195.9	14	0.286
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	17 %	15.17	3173	56.33	0.063
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	17 %	11.37	192.1	13.86	0.3
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	7.206	2951	54.32	0.129
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	4 %	3.299	80.51	8.973	0.707
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	7.491	3516	59.29	-0.04
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	4 %	3.656	641.4	25.33	-1.34
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	10.44	3100	55.68	0.085
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	8 %	6.542	157.5	12.55	0.426
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	9.332	3058	55.3	0.097
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	7 %	5.47	123.6	11.12	0.549
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	6.768	2893	53.79	0.146
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	3 %	2.914	73.68	8.583	0.731
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	5.094	2853	53.41	0.158
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	1 %	1.359	24.71	4.971	0.91
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	8.439	3144	56.07	0.072
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	5 %	4.606	244	15.62	0.111
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	7.357	3073	55.44	0.093
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	4 %	3.616	160.5	12.67	0.415
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	19 %	16.27	3236	56.89	0.045
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	18 %	12.35	252.5	15.89	0.08

======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23 %	19.17	3490	59.08	-0.03
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	23 %	15.29	448.4	21.18	-0.63
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	6.278	2907	53.92	0.142
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	3 %	2.39	48.31	6.95	0.824
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	5.038	2912	53.97	0.14
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	1 %	1.204	20.05	4.478	0.927
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	12.75	3262	57.12	0.037
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	12 %	8.703	178.9	13.38	0.348
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	12.66	3255	57.05	0.039
Exp x NIST	1 %	4.215	2820	53.11	0.167
NIST x Model	12 %	8.591	177.8	13.34	0.352

S1.3 Isochoric heat capacity (Cv)

Table S4: Evaluation of multiple ML models for $\boldsymbol{Cv}$ in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in J·mol^{-1}·K^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
KNeighborsRegressor	0.53	0.57	1.78
ExtraTreesRegressor	0.48	0.53	1.88
HistGradientBoostingRegressor	0.34	0.41	2.10
LGBMRegressor	0.34	0.41	2.10
XGBRegressor	0.33	0.40	2.12
NuSVR	0.33	0.39	2.12
SVR	0.33	0.39	2.12
RandomForestRegressor	0.32	0.38	2.14
GradientBoostingRegressor	0.32	0.38	2.14
DecisionTreeRegressor	0.31	0.38	2.15
ExtraTreeRegressor	0.31	0.37	2.16
BaggingRegressor	0.31	0.37	2.16
LinearSVR	0.30	0.37	2.16
AdaBoostRegressor	0.30	0.37	2.16
RANSACRegressor	0.29	0.36	2.18
SGDRegressor	0.29	0.35	2.19
HuberRegressor	0.28	0.35	2.19
OrthogonalMatchingPursuitCV	0.28	0.35	2.20
OrthogonalMatchingPursuit	0.28	0.35	2.20
LinearRegression	0.28	0.35	2.20
TransformedTargetRegressor	0.28	0.35	2.20
Lars	0.28	0.35	2.20
LassoLarsIC	0.28	0.35	2.20
RidgeCV	0.28	0.35	2.20
Ridge	0.28	0.35	2.20
BayesianRidge	0.28	0.35	2.20
PoissonRegressor	0.28	0.35	2.20
LarsCV	0.28	0.35	2.20
LassoLarsCV	0.28	0.35	2.20
ElasticNetCV	0.28	0.35	2.20
LassoCV	0.28	0.35	2.20
PassiveAggressiveRegressor	0.18	0.26	2.34
GammaRegressor	0.14	0.22	2.40
TweedieRegressor	0.14	0.22	2.40
ElasticNet	0.12	0.21	2.42
Lasso	0.09	0.17	2.48
LassoLars	0.09	0.17	2.48
DummyRegressor	-0.15	-0.04	2.77
MLPRegressor	-86.82	-78.45	24.27
GaussianProcessRegressor	-117.08	-105.83	28.14

KernelRidge	-148.30	-134.08	31.65

Table S5: ML performance metrics for predicting $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.767	2.784	1.669	0.42
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.587	0.732	0.856	0.675
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.647	2.366	1.538	0.507
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.468	0.457	0.676	0.797
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.797	2.924	1.71	0.39
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.622	0.877	0.937	0.611
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.65	2.366	1.538	0.507
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.485	0.473	0.687	0.79
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.632	2.401	1.55	0.5
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.481	0.439	0.663	0.805
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.471	1.927	1.388	0.598
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.365	0.225	0.474	0.9
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.794	3.373	1.837	0.297
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.651	1.46	1.208	0.352
======== GradientBoosting - CV = LOO ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.442	2.259	1.503	0.529
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.395	0.511	0.715	0.773
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.894	2.823	1.68	0.412
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.709	0.833	0.913	0.63
======== KNeighbors ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.313	0.966	0.983	0.799
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.386	0.398	0.631	0.823
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.928	2.818	1.679	0.413
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.72	0.833	0.913	0.63
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.368	4.762	2.182	0.007
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	4 %	1.148	2.238	1.496	0.006
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	3.554	56.971	7.548	-10.876
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	11 %	3.343	53.207	7.294	-22.621
======== RandomForest ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.533	1.958	1.399	0.592
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	1 %	0.396	0.257	0.507	0.886
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.823	2.645	1.626	0.449
Exp x NIST	2 %	0.446	1.815	1.347	0.622
NIST x Model	2 %	0.644	0.65	0.806	0.712
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.682	2.289	1.513	0.523
Exp x NIST	2 %	0.446	1.815	1.347	0.622

NIST x Model	2 %	0.532	0.497	0.705	0.78

S1.4 Joule-Thomson

No data

S1.5 Sound Speed

Table S6: Evaluation of multiple ML models for the Sound Speed ($m \cdot s^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
RandomForestRegressor	0.96	0.96	78.8
GradientBoostingRegressor	0.95	0.95	81.7
KNeighborsRegressor	0.95	0.95	85.9
ExtraTreesRegressor	0.94	0.94	88.5
BaggingRegressor	0.94	0.94	90.6
HistGradientBoostingRegressor	0.94	0.94	91.1
LGBMRegressor	0.94	0.94	93.4
DecisionTreeRegressor	0.93	0.93	96.2
XGBRegressor	0.93	0.93	101
ExtraTreeRegressor	0.87	0.88	132
TransformedTargetRegressor	0.82	0.82	160
LassoLarsCV	0.82	0.82	160
OrthogonalMatchingPursuitCV	0.82	0.82	160
Lars	0.82	0.82	160
LarsCV	0.82	0.82	160
LinearRegression	0.82	0.82	160
LassoLarsIC	0.82	0.82	160
BayesianRidge	0.82	0.82	160
HuberRegressor	0.82	0.82	160
Ridge	0.82	0.82	160
SGDRegressor	0.82	0.82	160
LassoLars	0.82	0.82	160
Lasso	0.82	0.82	160
PassiveAggressiveRegressor	0.81	0.82	160
LassoCV	0.81	0.82	160
RidgeCV	0.81	0.82	161
AdaBoostRegressor	0.78	0.78	176
ElasticNetCV	0.74	0.75	188
PoissonRegressor	0.71	0.72	199
ElasticNet	0.69	0.70	207
OrthogonalMatchingPursuit	0.56	0.57	247
TweedieRegressor	0.56	0.57	247
GammaRegressor	0.53	0.54	255
RANSACRegressor	0.25	0.27	322
SVR	0.14	0.16	346
NuSVR	0.07	0.09	360

DummyRegressor	-0.1	-0.08	391
LinearSVR	-1.75	-1.68	617
MLPRegressor	-4.04	-3.91	835
KernelRidge	-4.98	-4.83	910
GaussianProcessRegressor	-465.3	-453.6	8037

Table S7: ML performance metrics for predicting Sound Speed ($m \cdot s^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28 %	181.002	306997.5	554.074	-0.836
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	27 %	183.043	307716.2	554.722	-0.879
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	100.618	23858.62	154.462	0.857
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	21 %	102.51	25118.63	158.489	0.847
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28 %	181.145	307916.1	554.902	-0.841
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	27 %	183.186	308635.6	555.55	-0.885
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	100.642	23865.7	154.485	0.857
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	21 %	102.537	25127.27	158.516	0.847
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28 %	179.634	296238.9	544.278	-0.772
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	27 %	181.604	296970.6	544.95	-0.813
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	22 %	100.446	23955.64	154.776	0.857
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	21 %	102.131	25180.61	158.684	0.846
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	28 %	179.792	297302.2	545.254	-0.778
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	27 %	181.765	298034.6	545.925	-0.82
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	22 %	100.449	23956.25	154.778	0.857
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	21 %	102.134	25181.85	158.688	0.846
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	122.151	58987.45	242.873	0.647
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	15 %	111.526	54490.18	233.431	0.667
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	53.931	15642.76	125.071	0.906
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	8 %	46.587	11661.84	107.99	0.929
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17%	111.461	50287.8	224.249	0.699
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	14 %	103.403	46994.11	216.781	0.713
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	35.365	8888.332	94.278	0.947
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	7 %	34.951	8154.814	90.304	0.95
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	84.666	36437.55	190.886	0.782
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	12 %	80.359	34558.58	185.899	0.789
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	39.423	10453.04	102.24	0.937
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	8 %	38.429	9782.535	98.907	0.94
======== HistGradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	122.251	57687.52	240.182	0.655
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	15 %	114.356	53758.66	231.859	0.672

======== HistGradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	53.368	14492.59	120.385	0.913
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	9 %	52.543	13820.96	117.563	0.916
======== LGBM_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	19 %	123.934	54546.45	233.552	0.674
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	17 %	116.529	50920.59	225.656	0.689
======== LGBM_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	63.603	17066.08	130.637	0.898
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	10 %	61.464	15661.94	125.148	0.904
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42 %	498.978	5999080	2449.302	-34.876
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	40 %	493.877	5996560	2448.788	-35.616
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20%	105.446	29341.38	171.293	0.825
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	19 %	102.686	25974.8	161.167	0.841
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	16 %	104.841	46811.73	216.36	0.72
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	13 %	96.433	43288.82	208.06	0.736
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	39.406	9515.947	97.55	0.943
Exp x NIST	6 %	25.674	11763.2	108.458	0.93
NIST x Model	7. %	37.786	8351.04	91.384	0.949

S1.6 Density

Table S8: Evaluation of multiple ML models of the Density ($kg \cdot m^{-3}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

Model	R^2_{adj}	R^2	RMSE
GradientBoostingRegressor	0.78	0.78	31.9
BaggingRegressor	0.69	0.7	37.6
SGDRegressor	0.68	0.69	38.3
OrthogonalMatchingPursuitCV	0.68	0.69	38.3
LassoLarsCV	0.68	0.69	38.3
LassoLarsIC	0.68	0.69	38.3
LarsCV	0.68	0.69	38.3
Lars	0.68	0.69	38.3
LinearRegression	0.68	0.69	38.3
TransformedTargetRegressor	0.68	0.69	38.3
BayesianRidge	0.68	0.69	38.3
RidgeCV	0.68	0.69	38.3
Ridge	0.68	0.69	38.3
LassoCV	0.68	0.69	38.3
Lasso	0.68	0.68	38.5
LassoLars	0.68	0.68	38.5
ElasticNetCV	0.67	0.68	38.7
RandomForestRegressor	0.67	0.67	39.1
HistGradientBoostingRegressor	0.66	0.67	39.3
RANSACRegressor	0.66	0.66	39.6
LGBMRegressor	0.66	0.66	39.7
PassiveAggressiveRegressor	0.65	0.66	39.7
PoissonRegressor	0.65	0.66	40
HuberRegressor	0.64	0.65	40.3
KNeighborsRegressor	0.63	0.64	41.3
ElasticNet	0.58	0.59	44
OrthogonalMatchingPursuit	0.58	0.58	44
AdaBoostRegressor	0.57	0.58	44.3
SVR	0.57	0.58	44.5
NuSVR	0.56	0.57	44.6
ExtraTreesRegressor	0.56	0.57	44.7
DecisionTreeRegressor	0.51	0.52	47.3
TweedieRegressor	0.48	0.49	48.6
GammaRegressor	0.48	0.49	48.7
ExtraTreeRegressor	0.48	0.49	48.8
LinearSVR	0.47	0.48	49.1

XGBRegressor	0.02	0.04	67.1
DummyRegressor	-0.02	0	68.4
QuantileRegressor	-0.04	-0.02	69.1
MLPRegressor	-22.25	-21.79	326
KernelRidge	-30.07	-29.45	377
GaussianProcessRegressor	-601.9	-589.8	1661

Table S9: ML performance metrics for predicting density ($kg \cdot m^{-3}$) values in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	19.853	1386.499	37.236	0.631
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	5 %	16.915	751.658	27.416	0.763
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	16.373	1072.103	32.743	0.715
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	4 %	13.464	447.311	21.15	0.859
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	19.888	1389.957	37.282	0.63
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	5 %	16.95	755.362	27.484	0.761
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	16.384	1072.168	32.744	0.715
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	4 %	13.476	447.528	21.155	0.859
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	13.246	1143.073	33.809	0.696
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	3 %	10.535	479.084	21.888	0.849
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	9.716	789.996	28.107	0.79
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	2 %	6.881	140.092	11.836	0.956

======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	11.348	958.675	30.962	0.745
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	3 %	8.512	301.341	17.359	0.905
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	7.753	763.241	27.627	0.797
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	2 %	4.927	122.223	11.055	0.961
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	9.792	911.935	30.198	0.757
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	2 %	7.062	257.33	16.041	0.919
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	7.268	773.878	27.819	0.794
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	1 %	4.508	124.334	11.151	0.961
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	14.352	1033.582	32.149	0.725
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	4 %	11.83	379.138	19.471	0.88
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	12.921	1018.795	31.919	0.729
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	3 %	10.243	376.958	19.415	0.881
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	8.163	773.569	27.813	0.794
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	2 %	5.315	132.219	11.499	0.958
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23 %	73.779	22211.52	149.035	-4.912
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	18 %	71.66	21733.1	147.422	-5.865
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	18.934	1161.596	34.082	0.691

Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	5 %	16.717	565.798	23.787	0.821
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	19.086	1335.683	36.547	0.645
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	5 %	16.51	710.639	26.658	0.776
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	13.952	908.762	30.146	0.758
Exp x NIST	6 %	4.122	695.778	26.378	0.815
NIST x Model	4 %	11.604	367.352	19.166	0.884

S1.7 Volume

Table S10: Evaluation of multiple ML models to the volume ($m^3 \cdot kg^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
BaggingRegressor	0.27	0.29	0
RandomForestRegressor	0.22	0.24	0
NuSVR	0.04	0.06	0
LinearSVR	0.04	0.06	0
LarsCV	0.03	0.05	0
LinearRegression	0.03	0.05	0
Lars	0.03	0.05	0
LassoLarsCV	0.03	0.05	0
LassoLarsIC	0.03	0.05	0
TransformedTargetRegressor	0.03	0.05	0
OrthogonalMatchingPursuitCV	0.03	0.05	0
LassoCV	0.03	0.05	0
ElasticNetCV	0.03	0.05	0
Ridge	0.03	0.05	0
BayesianRidge	0.03	0.05	0
RidgeCV	0.03	0.05	0
SGDRegressor	0.03	0.05	0
AdaBoostRegressor	0.03	0.05	0
GradientBoostingRegressor	0.02	0.04	0
OrthogonalMatchingPursuit	0.01	0.03	0
TweedieRegressor	0.01	0.03	0
GammaRegressor	0.01	0.03	0
HuberRegressor	0.01	0.03	0
RANSACRegressor	0	0.02	0
PoissonRegressor	-0.02	0	0
DummyRegressor	-0.02	0	0
Lasso	-0.02	0	0
LassoLars	-0.02	0	0
ElasticNet	-0.02	0	0
LGBMRegressor	-0.04	-0.02	0
QuantileRegressor	-0.04	-0.02	0
XGBRegressor	-0.05	-0.03	0
HistGradientBoostingRegressor	-0.08	-0.06	0
KNeighborsRegressor	-0.29	-0.27	0
ExtraTreesRegressor	-0.53	-0.5	0
DecisionTreeRegressor	-0.89	-0.85	0

KernelRidge	-1.06	-1.02	0
PassiveAggressiveRegressor	-1.1	-1.06	0
ExtraTreeRegressor	-2.87	-2.79	0.01
SVR	-22.36	-21.9	0.01
MLPRegressor	-86.41	-84.66	0.03
GaussianProcessRegressor	-2465	-2415	0.14

Table S11: ML performance metrics for predicting the volume ($m^3 \cdot kg^{-1}$) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	0.001	0	0.002	-0.038
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	17 %	0	0	0.001	-0.295
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	0.001	0	0.002	-0.008
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	17 %	0	0	0.001	-0.135
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	0.001	0	0.002	-0.009
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	14 %	0	0	0.001	-0.094
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0	0	0.002	0.058
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	10 %	0	0	0	0.449
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	0.001	0	0.002	-0.028
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	16 %	0	0	0.001	-0.204
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	16 %	0.001	0	0.002	-0.004
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	15 %	0	0	0.001	-0.057
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	0	0	0.002	0.001
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	13 %	0	0	0.001	-0.019
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0	0	0.002	0.055
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	10 %	0	0	0	0.429
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0	0	0.002	-0.053
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	4 %	0	0	0.001	-0.449
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0	0	0.002	0.071
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	2 %	0	0	0	0.772
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0	0	0.002	-0.003
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	10 %	0	0	0.001	-0.004
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	0	0	0.002	0.057
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	7 %	0	0	0	0.37
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	0	0	0.002	-0.112
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	8 %	0	0	0.001	-1.074
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	0	0	0.002	-0.051
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	6 %	0	0	0.001	-0.467
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	304 %	0.008	0	0.012	-37.07
Exp x NIST	1 %	0	0	0.002	0.079

NIST x Model	305 %	0.008	0	0.012	-375.291
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	391 %	0.01	0.001	0.031	-251.304
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	392 %	0.01	0.001	0.031	-2538.76
======== NuSVR_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	0	0	0.002	0.042
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	7 %	0	0	0	0.396
======== NuSVR_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0	0	0.002	0.056
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	5 %	0	0	0	0.669
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	0	0	0.002	-0.098
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	8 %	0	0	0.001	-0.916
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0	0	0.002	0.008
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	6 %	0	0	0.001	-0.373
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	0.001	0	0.002	-0.067
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	15 %	0	0	0.001	-0.564
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	0	0	0.002	0.057
Exp x NIST	1 %	0	0	0.002	0.079
NIST x Model	12 %	0	0	0.001	-0.057

S1.8 Enthalpy

Table S12: Evaluation of multiple ML models for the enthalpy (kJ·mol^{-1}) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in kJ·mol^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
GradientBoostingRegressor	0.98	0.98	0.25
LGBMRegressor	0.98	0.98	0.27
HistGradientBoostingRegressor	0.98	0.98	0.27
XGBRegressor	0.97	0.98	0.28
NuSVR	0.96	0.96	0.35
BaggingRegressor	0.96	0.96	0.35
SVR	0.96	0.96	0.35
ExtraTreesRegressor	0.96	0.96	0.36
SGDRegressor	0.96	0.96	0.36
Ridge	0.96	0.96	0.36
ElasticNetCV	0.96	0.96	0.36
RidgeCV	0.96	0.96	0.36
BayesianRidge	0.96	0.96	0.36
TransformedTargetRegressor	0.96	0.96	0.36
OrthogonalMatchingPursuitCV	0.96	0.96	0.36
LinearRegression	0.96	0.96	0.36
LassoLarsIC	0.96	0.96	0.36
LassoLarsCV	0.96	0.96	0.36
LarsCV	0.96	0.96	0.36
Lars	0.96	0.96	0.36
LassoCV	0.96	0.96	0.36
HuberRegressor	0.96	0.96	0.36
LinearSVR	0.96	0.96	0.36
RandomForestRegressor	0.96	0.96	0.36
DecisionTreeRegressor	0.95	0.96	0.37
ExtraTreeRegressor	0.95	0.96	0.37
RANSACRegressor	0.95	0.96	0.37
OrthogonalMatchingPursuit	0.95	0.95	0.37
MLPRegressor	0.95	0.95	0.38
GaussianProcessRegressor	0.95	0.95	0.4
AdaBoostRegressor	0.94	0.95	0.41
KNeighborsRegressor	0.94	0.94	0.42
PassiveAggressiveRegressor	0.91	0.91	0.53
PoissonRegressor	0.89	0.89	0.58
TweedieRegressor	0.72	0.72	0.92
ElasticNet	0.68	0.69	0.99

Lasso	0.6	0.61	1.1
LassoLars	0.6	0.61	1.1
DummyRegressor	-0.04	-0.01	1.77
QuantileRegressor	-0.1	-0.06	1.81
KernelRidge	-1.05	-0.99	2.48

Table S13: ML performance metrics for predicting enthalpy (kJ·mol^{-1}) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in kJ·mol^{-1} are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	539937585917565 %	0.172	0.138	0.371	0.952
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	251 %	0.519	0.292	0.541	0.902
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	308646208535984 %	0.155	0.11	0.332	0.962
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	255 %	0.531	0.301	0.549	0.899
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1532755325052460 %	0.16	0.131	0.362	0.955
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	226 %	0.521	0.291	0.54	0.902
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1200984837455310 %	0.143	0.105	0.323	0.964
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	232 %	0.525	0.292	0.54	0.902
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	321522735478706 %	0.167	0.124	0.353	0.957
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	259 %	0.535	0.309	0.556	0.897
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	377864331591738 %	0.159	0.115	0.338	0.96
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	256 %	0.533	0.304	0.551	0.898
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	1373393186827640 %	0.148	0.117	0.343	0.959
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	232 %	0.532	0.301	0.549	0.899
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1376417407648350 %	0.144	0.108	0.328	0.963
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	233 %	0.531	0.299	0.547	0.9
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6365269990061 %	0.093	0.103	0.321	0.964
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	263 %	0.563	0.324	0.569	0.891
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5064838486714 %	0.065	0.06	0.246	0.979
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	264 %	0.577	0.346	0.589	0.884
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9833999915821 %	0.084	0.094	0.307	0.968
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	262 %	0.558	0.315	0.561	0.894
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2532419243358 %	0.053	0.056	0.236	0.981
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	265 %	0.582	0.35	0.592	0.883
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28639152569949 %	0.15	0.202	0.45	0.93
Exp x NIST	5145114807847790 %	0.59	0.364	0.603	0.875
NIST x Model	270%	0.595	0.364	0.604	0.878
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7168864917186 %	0.036	0.033	0.181	0.989
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	264%	0.583	0.357	0.597	0.88
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7893639014686%	0.095	0.106	0.326	0.963
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	261%	0.558	0.318	0.564	0.893

======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3068180598995%	0.076	0.091	0.301	0.969
Exp x NIST	5145114807847790	0.59	0.364	0.603	0.875
NIST x Model	261 %	0.561	0.321	0.566	0.892
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	275578987615547%	0.262	0.151	0.389	0.948
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	261%	0.536	0.347	0.589	0.884
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1689609359106390%	0.302	0.203	0.45	0.93
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	260%	0.558	0.394	0.628	0.868
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7550715971002%	0.085	0.1	0.316	0.965
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	262%	0.559	0.316	0.562	0.894
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3598659003162%	0.059	0.059	0.242	0.98
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	262%	0.562	0.32	0.566	0.893
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	334108698025279%	0.308	0.275	0.524	0.905
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	267%	0.523	0.343	0.586	0.885
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	283268126213326%	0.09	0.024	0.154	0.992
Exp x NIST	5145114807847790%	0.59	0.364	0.603	0.875
NIST x Model	277%	0.568	0.338	0.581	0.887

S1.9 Viscosity

Table S14: Evaluation of multiple ML models to the Viscosity (µPa·s) for the liquid phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in µPa·s are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreesRegressor	0.9	0.91	18.5
GradientBoostingRegressor	0.88	0.89	20.1
RandomForestRegressor	0.83	0.84	23.9
BaggingRegressor	0.81	0.83	24.9
AdaBoostRegressor	0.8	0.82	25.6
DecisionTreeRegressor	0.8	0.81	26
XGBRegressor	0.72	0.75	30.3
KNeighborsRegressor	0.72	0.74	30.6
ExtraTreeRegressor	0.71	0.74	31
LGBMRegressor	0.65	0.69	33.9
HistGradientBoostingRegressor	0.64	0.68	34.3
HuberRegressor	0.61	0.64	36
PassiveAggressiveRegressor	0.6	0.64	36.2
PoissonRegressor	0.59	0.63	36.8
SGDRegressor	0.59	0.63	36.9
LassoLarsIC	0.59	0.63	36.9
LarsCV	0.59	0.63	36.9
Lars	0.59	0.63	36.9
LassoLarsCV	0.59	0.63	36.9
OrthogonalMatchingPursuitCV	0.59	0.63	36.9
LinearRegression	0.59	0.63	36.9
TransformedTargetRegressor	0.59	0.63	36.9
RidgeCV	0.59	0.63	37
LassoCV	0.59	0.63	37
BayesianRidge	0.59	0.62	37
Ridge	0.59	0.62	37
Lasso	0.58	0.62	37.1
LassoLars	0.58	0.62	37.1
ElasticNetCV	0.58	0.62	37.2
GaussianProcessRegressor	0.56	0.6	38
RANSACRegressor	0.5	0.54	40.8
ElasticNet	0.48	0.53	41.5
GammaRegressor	0.41	0.46	44.3
TweedieRegressor	0.38	0.44	45.2
OrthogonalMatchingPursuit	0.15	0.23	53
NuSVR	0.05	0.14	56.1

SVR	0.01	0.1	57.3
DummyRegressor	-0.16	-0.06	62
QuantileRegressor	-0.23	-0.12	63.9
LinearSVR	-0.29	-0.17	65.4
MLPRegressor	-3.69	-3.26	125
KernelRidge	-3.96	-3.51	128

Table S15: ML performance metrics for predicting viscosity (µPa·s) in the liquid phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in µPa·s are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43%	29.449	1721.404	41.49	0.585
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	22%	19.503	686.788	26.207	0.767
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	38 %	25.697	1303.809	36.108	0.686
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	21%	19.289	701.219	26.481	0.762
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43%	29.417	1719.991	41.473	0.585
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	21%	19.499	688.089	26.231	0.766
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	38%	25.684	1303.555	36.105	0.686
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	21%	19.296	703.132	26.517	0.761
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42%	28.81	1666.728	40.826	0.598
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	21%	18.692	633.598	25.171	0.785
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	39%	25.752	1319.146	36.32	0.682
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	21%	19.16	698.483	26.429	0.763
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42%	28.784	1665.875	40.815	0.598
Exp x NIST	29%	21.334	2050.595	45.284	0.506
NIST x Model	20%	18.69	635.359	25.206	0.784
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	39 %	25.737	1318.966	36.318	0.682
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	21 %	19.165	700.412	26.465	0.762
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37 %	21.292	1435.613	37.889	0.654
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	27 %	24.092	1232.395	35.105	0.581
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	6.633	405.098	20.127	0.902
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	23 %	22.599	2046.324	45.236	0.305
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33 %	17.89	971.999	31.177	0.766
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	22 %	19.722	802.778	28.333	0.727
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	4.925	168.25	12.971	0.959
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	21 %	20.701	1728.919	41.58	0.413
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	29 %	13.531	670.806	25.9	0.838
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	21 %	19.206	1006.692	31.728	0.658
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	5.79	338.176	18.39	0.918
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	23 %	22.389	1980.447	44.502	0.327
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42 %	26.619	1441.714	37.97	0.652
Exp x NIST	29 %	21.334	2050.595	45.284	0.506

NIST x Model	29 %	24.668	1034.969	32.171	0.648
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	33.911	1841.628	42.914	0.556
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	31 %	30.992	1850.965	43.023	0.371
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	41 %	26.703	1405.696	37.493	0.661
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	25 %	23.486	1163.438	34.109	0.605
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	34 %	18.249	895.748	29.929	0.784
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	26 %	25.278	1349.849	36.74	0.541
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	6.648	405.282	20.132	0.902
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	23 %	22.621	2046.498	45.238	0.305
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	31 %	14.272	664.346	25.775	0.84
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	28 %	26.797	1854.556	43.065	0.37
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23 %	10.82	381.117	19.522	0.908
Exp x NIST	29 %	21.334	2050.595	45.284	0.506
NIST x Model	26 %	24.749	1824.836	42.718	0.38

S2. Vapor Phase

S2.1 Best metrics

On Table S16, the units of MAE and RMSE are reported in the same units as the target property, while MSE carries squared units. For instance, when predicting density ($kg \cdot m^{-3}$) or sound speed ($m \cdot s^{-1}$), MAE and RMSE are expressed in $kg \cdot m^{-3}$ and $m \cdot s^{-1}$, respectively, while MSE carries squared units, such as $(kg \cdot m^{-3})^2$ or $(m \cdot s^{-1})^2$. The MAPE, in contrast, is unitless and expressed as a percentage. The R^2 metric is also unitless

Tables even-numbered from Table S18 to Table S32 presents all the ML performance metrics for predicting the corresponding investigated property in vapor phase. Data in red represents the best model for each property.

Table S16: ML performance metrics for the best-performing models for predicting various thermophysical properties in the vapor phase, including density ($kg \cdot m^{-3}$), Volume ($m^3 \cdot kg^{-1}$), enthalpy ($kJ \cdot mol^{-1}$), $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$), $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$), sound speed ($m \cdot s^{-1}$), Joule-Thomson Coefficient ($K \cdot MPa^{-1}$), and viscosity (µPa·s). The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in the respective property units are presented.

Cp – Random Forest – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	19 %	28.298	19309.547	138.959	0.036
Exp x NIST	2 %	18.556	17686.113	132.989	0.117
NIST x Model	18 %	10.818	907.213	30.12	0.178
Cv – ExtraTrees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	12 %	3.340	17.672	4.204	-0.488
Exp x NIST	3 %	0.662	0.656	0.810	0.945
NIST x Model	9 %	2.678	14.589	3.820	-0.785
Joule-Thomson – Extra Trees – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	3 %	0.13	0.038	0.195	0.978
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	4 %	0.143	0.028	0.169	0.981
Sound Speed – GradientBoosting – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	26 %	131.632	56130.553	236.919	-0.29
Exp x NIST	21 %	140.145	65033.991	255.018	-0.494
NIST x Model	33 %	107.677	41905.553	204.708	-1.223
Density – GradientBoosting – CV = LOO					

Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	22 %	7.144	471.201	21.707	0.678
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	21 %	4.625	148.901	12.203	0.797
Volume – Extra Trees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	18 %	0.008	0.001	0.034	0.993
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	8 %	0.007	0.001	0.032	0.994
Enthalpy – Decision Tree – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	63 %	0.542	3.83	1.957	0.232
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	7 %	0.587	0.599	0.774	0.784
Viscosity – Extra Trees – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	5 %	1.311	80.682	8.982	-0.05
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	4 %	0.545	6.48	2.546	0.332

S2.2 Isobaric heat capacity (Cp)

Table S17: Evaluation of multiple ML models for $\boldsymbol{Cp}$ in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in J·mol^{-1}·K^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreeRegressor	0.96	0.96	53.35
DecisionTreeRegressor	0.96	0.96	53.36
GradientBoostingRegressor	0.96	0.96	53.44
AdaBoostRegressor	0.95	0.96	53.90
ExtraTreesRegressor	0.95	0.96	54.93
BaggingRegressor	0.80	0.81	113.74
RandomForestRegressor	0.75	0.77	125.34
KNeighborsRegressor	0.25	0.29	218.60
HistGradientBoostingRegressor	0.18	0.23	228.78
LGBMRegressor	0.18	0.23	228.78
PoissonRegressor	-0.04	0.02	257.14
SGDRegressor	-0.06	0.00	259.86
LassoLarsIC	-0.06	0.00	259.87
TransformedTargetRegressor	-0.06	0.00	259.87
Lars	-0.06	0.00	259.87
LarsCV	-0.06	0.00	259.87
OrthogonalMatchingPursuitCV	-0.06	0.00	259.87
LinearRegression	-0.06	0.00	259.87
LassoLarsCV	-0.06	0.00	259.87
LassoCV	-0.06	0.00	259.87
Ridge	-0.06	0.00	259.90
Lasso	-0.07	0.00	260.10
LassoLars	-0.07	0.00	260.10
RidgeCV	-0.07	0.00	260.16
OrthogonalMatchingPursuit	-0.07	-0.00	260.25
ElasticNetCV	-0.07	-0.00	260.81
BayesianRidge	-0.07	-0.01	260.87
ElasticNet	-0.08	-0.01	261.52
TweedieRegressor	-0.08	-0.02	262.35
GammaRegressor	-0.09	-0.02	262.91
XGBRegressor	-0.10	-0.03	264.71
DummyRegressor	-0.11	-0.04	265.76
NuSVR	-0.11	-0.04	265.79
SVR	-0.11	-0.04	265.81
PassiveAggressiveRegressor	-0.12	-0.05	266.16
HuberRegressor	-0.12	-0.05	267.03

LinearSVR	-0.13	-0.06	268.05
RANSACRegressor	-0.14	-0.07	268.76
KernelRidge	-0.20	-0.13	276.29
MLPRegressor	-0.22	-0.14	277.78
GaussianProcessRegressor	-15583.47	-14609.44	31453.98

Table S18: ML performance metrics for predicting $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	98%	60.23	24590	156.8	-0.23
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	97%	42.85	5861	76.56	-4.31
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	98%	61.47	20116	141.8	-0.01
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	96%	44.44	2981	54.59	-1.7
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	99%	60.59	24666	157.1	-0.23
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	98%	43.19	5940	77.07	-4.38
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	98%	61.61	20114	141.8	-0.01
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	96%	44.58	2986	54.65	-1.7
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	96%	60.37	22135	148.8	-0.11
Exp x NIST	2%	18.56	17686	133	0.117

NIST x Model	95%	42.96	3297	57.42	-1.99
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	75%	51.35	19612	140	0.02
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	73%	33.95	1949	44.15	-0.77
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	97%	60.59	22179	148.9	-0.11
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	95%	43.18	3338	57.78	-2.02
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	75%	51.49	19612	140	0.02
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	73%	34.08	1954	44.21	-0.77
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	46%	41.18	22617	150.4	-0.13
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	44%	23.66	3846	62.02	-2.48
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4%	5.786	1032	32.13	0.948
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	20%	19.99	14382	119.9	-12
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	29%	33.92	20326	142.6	-0.02
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	28%	16.5	1787	42.27	-0.62
======== ExtraTreesRegressor - CV = LOO ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	32	31.75	13331	115.5	0.334
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	35%	21.73	2961	54.41	-1.68
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20%	29.43	23508	153.3	-0.17
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	19%	12.12	5060	71.13	-3.58
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17%	13.46	5979	77.32	0.701
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	34%	27.93	19431	139.4	-16.6
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23%	31.1	20607	143.6	-0.03
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	22%	13.64	1823	42.7	-0.65
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	34%	21.84	4707	68.61	0.765
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	47%	30.5	12076	109.9	-9.94
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	56%	43.14	20626	143.6	-0.03
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	54%	25.66	1589	39.86	-0.44
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	84%	56.81	23768	154.2	-0.19

Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	83%	39.52	3979	63.08	-2.6
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	19%	28.3	19310	139	0.036
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	18%	10.82	907.2	30.12	0.178
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37	31.61	14741	121.4	0.264
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	40%	22.78	5490	74.09	-3.97
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33%	34.1	20051	141.6	-0
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	31%	16.58	1235	35.15	-0.12
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	45%	37.62	16558	128.7	0.173
Exp x NIST	2%	18.56	17686	133	0.117
NIST x Model	44%	23.1	1974	44.43	-0.79

S2.3 Isochoric heat capacity (Cv)

Table S19: Evaluation of multiple ML models for $\boldsymbol{Cv}$ in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in J·mol^{-1}·K^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
AdaBoostRegressor	NaN	NaN	0.87
BaggingRegressor	NaN	NaN	3.31
BayesianRidge	NaN	NaN	0.48
DecisionTreeRegressor	NaN	NaN	2.18
DummyRegressor	NaN	NaN	3.09
ElasticNet	NaN	NaN	1.71
ExtraTreeRegressor	NaN	NaN	0.87
ExtraTreesRegressor	NaN	NaN	0.87
GammaRegressor	NaN	NaN	1.78
GaussianProcessRegressor	NaN	NaN	0.97
GradientBoostingRegressor	NaN	NaN	0.39
HistGradientBoostingRegressor	NaN	NaN	3.09
HuberRegressor	NaN	NaN	0.48
KernelRidge	NaN	NaN	26.50
Lars	NaN	NaN	0.48
Lasso	NaN	NaN	1.37
LassoLars	NaN	NaN	1.37
LinearRegression	NaN	NaN	0.48
LinearSVR	NaN	NaN	21.64
MLPRegressor	NaN	NaN	19.94
NuSVR	NaN	NaN	3.12
OrthogonalMatchingPursuit	NaN	NaN	0.67
PassiveAggressiveRegressor	NaN	NaN	0.51
PoissonRegressor	NaN	NaN	0.55
RANSACRegressor	NaN	NaN	0.48
RandomForestRegressor	NaN	NaN	2.85
Ridge	NaN	NaN	1.24
RidgeCV	NaN	NaN	2.53
SGDRegressor	NaN	NaN	0.20
SVR	NaN	NaN	1.69
TransformedTargetRegressor	NaN	NaN	0.48
TweedieRegressor	NaN	NaN	1.88
XGBRegressor	NaN	NaN	2.18
LGBMRegressor	NaN	NaN	3.09

Table S20: ML performance metrics for predicting $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	211%	55.28	6015.151	77.557	-505.533
Exp x NIST	3%	0.662	0.656	0.81	0.945
NIST x Model	206%	54.665	5989.066	77.389	-731.565
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	24%	6.418	48.935	6.995	-3.121
Exp x NIST	3%	0.662	0.656	0.81	0.945
NIST x Model	21%	5.756	39.354	6.273	-3.814
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	143%	37.585	2575.279	50.747	-215.863
Exp x NIST	3%	0.662	0.656	0.81	0.945
NIST x Model	139%	36.97	2555.747	50.554	-311.611
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	24%	6.424	49.062	7.004	-3.131
Exp x NIST	3%	0.662	0.656	0.81	0.945
NIST x Model	21%	5.763	39.468	6.282	-3.828
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14%	3.852	20.136	4.487	-0.696
Exp x NIST	3%	0.662	0.656	0.81	0.945
NIST x Model	11 %	3.237	16.067	4.008	-0.965
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	3.34	17.672	4.204	-0.488
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	9 %	2.678	14.589	3.82	-0.785
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	3.473	19.897	4.461	-0.676
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	10 %	2.811	15.512	3.939	-0.897
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	4.018	21.193	4.604	-0.785

Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	12 %	3.356	16.666	4.082	-1.039
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	4.177	22.33	4.725	-0.88
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	12 %	3.562	17.279	4.157	-1.114
======== KNeighbors ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	3.767	21.111	4.595	-0.778
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	11 %	3.152	16.195	4.024	-0.981
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	4.177	22.33	4.725	-0.88
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	12 %	3.562	17.279	4.157	-1.114
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	41 %	11.374	164.666	12.832	-12.866
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	38 %	10.759	157.268	12.541	-18.237
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	22 %	6.404	60.714	7.792	-4.113
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	24 %	6.872	62.791	7.924	-6.68
======== RandomForest ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	3.661	19.555	4.422	-0.647
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	11 %	3.12	15.312	3.913	-0.873
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	4.177	22.33	4.725	-0.88
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	12 %	3.562	17.279	4.157	-1.114
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	3.767	21.111	4.595	-0.778
Exp x NIST	3 %	0.662	0.656	0.81	0.945
NIST x Model	11 %	3.152	16.195	4.024	-0.981

S2.4 Joule-Thomson

Table S21: Evaluation of multiple ML models for the Joule-Thomson Coefficient ($K \cdot MPa^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $K \cdot MPa^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
GaussianProcessRegressor	0.99	0.99	0.08
GradientBoostingRegressor	0.98	0.99	0.09
XGBRegressor	0.98	0.99	0.1
ExtraTreesRegressor	0.97	0.98	0.12
SVR	0.97	0.98	0.12
DecisionTreeRegressor	0.97	0.98	0.12
ExtraTreeRegressor	0.96	0.98	0.14
NuSVR	0.96	0.98	0.14
AdaBoostRegressor	0.95	0.97	0.15
RandomForestRegressor	0.94	1	0.17
BaggingRegressor	0.93	1	0.19
LinearSVR	0.86	0.9	0.26
SGDRegressor	0.84	0.9	0.28
HuberRegressor	0.84	0.9	0.28
RANSACRegressor	0.81	0.9	0.31
LassoLarsCV	0.8	0.9	0.31
Lars	0.8	0.9	0.31
OrthogonalMatchingPursuitCV	0.8	0.9	0.31
LarsCV	0.8	0.9	0.31
LassoLarsIC	0.8	0.9	0.31
TransformedTargetRegressor	0.8	0.9	0.31
LinearRegression	0.8	0.9	0.31
BayesianRidge	0.8	0.9	0.31
LassoCV	0.8	0.9	0.32
ElasticNetCV	0.79	0.9	0.32
RidgeCV	0.78	0.9	0.32
Ridge	0.78	0.9	0.32
PoissonRegressor	0.77	0.9	0.34
OrthogonalMatchingPursuit	0.75	0.9	0.35
KNeighborsRegressor	0.6	0.8	0.44
PassiveAggressiveRegressor	0.54	0.7	0.47
GammaRegressor	0.37	0.6	0.56
MLPRegressor	0.31	0.6	0.58
TweedieRegressor	0.25	0.6	0.61
ElasticNet	0.1	0.5	0.66
LassoLars	-0.37	0.2	0.82

Lasso	-0.37	0.2	0.82
QuantileRegressor	-0.77	-0.1	0.93
LGBMRegressor	-1.09	-0.3	1.01
DummyRegressor	-1.09	-0.3	1.01
HistGradientBoostingRegressor	-1.09	-0.3	1.01
KernelRidge	-27.6	-16	3.73

Table S22: ML performance metrics for predicting Joule-Thomson Coefficient ($K \cdot MPa^{-1}$) for the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $K \cdot MPa^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.42	0.26	0.509	0.852
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	8 %	0.296	0.121	0.348	0.917
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	0.343	0.166	0.408	0.905
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	7 %	0.227	0.074	0.271	0.95
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	0.427	0.251	0.501	0.858
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	9 %	0.323	0.14	0.374	0.905
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.358	0.175	0.419	0.9
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	8 %	0.284	0.114	0.337	0.922
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.424	0.258	0.508	0.853
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	9 %	0.298	0.12	0.346	0.918
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.385	0.207	0.455	0.882
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	8 %	0.262	0.093	0.306	0.936
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	0.424	0.268	0.518	0.848
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	9 %	0.316	0.148	0.385	0.899
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.38	0.219	0.468	0.876
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	8 %	0.276	0.12	0.346	0.918
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.176	0.065	0.255	0.963
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	6 %	0.214	0.078	0.279	0.947
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.079	0.018	0.134	0.99
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	4 %	0.142	0.033	0.182	0.977
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.13	0.038	0.195	0.978
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	4 %	0.143	0.028	0.169	0.981
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.067	0.012	0.112	0.993
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	4 %	0.168	0.042	0.206	0.971
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.193	0.08	0.283	0.955
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	6 %	0.219	0.082	0.287	0.944
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.123	0.043	0.207	0.976
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	4 %	0.162	0.067	0.259	0.954
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	63 %	2.546	12.688	3.562	-6.21

Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	63 %	2.442	12.192	3.492	-7.323
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	1.419	3.663	1.914	-1.082
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	36 %	1.359	3.325	1.823	-1.27
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	0.345	0.222	0.471	0.874
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	9 %	0.355	0.165	0.406	0.887
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0.261	0.173	0.415	0.902
Exp x NIST	4 %	0.18	0.059	0.242	0.967
NIST x Model	7 %	0.259	0.101	0.318	0.931

S2.5 Sound Speed

Table S23: Evaluation of multiple ML models for the Sound Speed ($m \cdot s^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
GradientBoostingRegressor	0.86	0.9	67.2
RandomForestRegressor	0.77	0.8	86.1
ExtraTreesRegressor	0.73	0.7	93.5
HistGradientBoostingRegressor	0.73	0.7	93.8
DecisionTreeRegressor	0.71	0.7	95.8
BaggingRegressor	0.71	0.7	96.9
AdaBoostRegressor	0.7	0.7	97.4
LGBMRegressor	0.7	0.7	98.8
ExtraTreeRegressor	0.66	0.7	104
XGBRegressor	0.64	0.7	107
KNeighborsRegressor	0.6	0.6	114
LassoCV	0.23	0.3	157
LassoLars	0.23	0.3	157
Lasso	0.23	0.3	157
Lars	0.23	0.3	157
LarsCV	0.23	0.3	157
LassoLarsCV	0.23	0.3	157
LassoLarsIC	0.23	0.3	157
OrthogonalMatchingPursuitCV	0.23	0.3	157
TransformedTargetRegressor	0.23	0.3	157
LinearRegression	0.23	0.3	157
Ridge	0.23	0.3	157
SGDRegressor	0.23	0.3	157
BayesianRidge	0.23	0.3	157
RidgeCV	0.23	0.3	157
ElasticNetCV	0.23	0.3	157
HuberRegressor	0.23	0.3	157
PoissonRegressor	0.22	0.3	158
OrthogonalMatchingPursuit	0.22	0.2	159
ElasticNet	0.2	0.2	160
TweedieRegressor	0.16	0.2	164
GammaRegressor	0.16	0.2	164
NuSVR	0.08	0.1	172
SVR	0.04	0.1	175
DummyRegressor	-0.04	0	182
PassiveAggressiveRegressor	-0.38	-0.3	210

RANSACRegressor	-0.79	-0.7	239
LinearSVR	-1.98	-1.9	309
MLPRegressor	-6.36	-6.1	486
KernelRidge	-7.62	-7.3	525
GaussianProcessRegressor	-1065	-1027.97	5844

Table S24: ML performance metrics for predicting the Sound Speed ($m \cdot s^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42 %	180.846	47072.74	216.963	-0.081
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	56 %	184.829	45266.01	212.758	-1.401
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37 %	154.49	34369.91	185.391	0.21
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	57 %	186.482	46788.95	216.308	-1.482
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	42 %	180.855	47020.03	216.841	-0.08
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	56 %	185.134	45378.96	213.023	-1.407
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37 %	154.643	34443.65	185.59	0.209
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	57 %	186.442	46773.71	216.272	-1.481
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43 %	188.317	50631.02	225.013	-0.163
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	53 %	178.724	42575.56	206.338	-1.258
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	155.172	34529.15	185.82	0.207
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	53 %	174.402	41397.53	203.464	-1.196
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	43 %	188.243	50595.03	224.933	-0.162
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	53 %	178.765	42615.87	206.436	-1.261
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	155.162	34527.9	185.817	0.207
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	53 %	174.455	41442.15	203.573	-1.198
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	25 %	122.548	46836.72	216.418	-0.076
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	36 %	115.575	44220.49	210.287	-1.346
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	50.965	23589.09	153.587	0.458
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	50 %	154.992	66958.23	258.763	-2.552
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	29 %	137.16	47900.58	218.862	-0.101
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	39 %	127.815	41326.36	203.289	-1.192
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	72.088	19882.53	141.005	0.543
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	50 %	155.336	55741.24	236.096	-1.957
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	26 %	131.632	56130.55	236.919	-0.29
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	33 %	107.677	41905.55	204.708	-1.223
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	63.656	20933.53	144.684	0.519
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	47 %	147.63	55377.41	235.324	-1.938
======== HistGradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	26 %	124.94	42986.81	207.333	0.012
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	39 %	124.981	41401.92	203.475	-1.196

======== HistGradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	62.702	17621.92	132.748	0.595
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	52 %	160.189	60515.66	245.999	-2.21
======== LGBM_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	25 %	122.853	42903.12	207.131	0.014
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	39 %	126.152	42376.24	205.855	-1.248
======== LGBM_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	16 %	66.096	17211.95	131.194	0.605
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	51 %	156.993	57419.11	239.623	-2.046
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	61 %	287.583	116072.5	340.694	-1.667
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	46 %	169.5	54515.88	233.486	-1.892
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	35 %	152.145	36079.08	189.945	0.171
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	51 %	162.526	39815.51	199.538	-1.112
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	25 %	122.462	47130.65	217.096	-0.083
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	39 %	124.477	46349.66	215.29	-1.459
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	58.005	19071.69	138.1	0.562
Exp x NIST	21 %	140.145	65033.99	255.018	-0.494
NIST x Model	50 %	153.574	59894.49	244.734	-2.177

S2.6 Density

Table S25: Evaluation of multiple ML models for the Density ($kg \cdot m^{-3}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

Model	R^2_{adj}	R^2	RMSE
GradientBoostingRegressor	0.99	1	3.85
XGBRegressor	0.99	1	4.39
ExtraTreesRegressor	0.98	1	5.89
ExtraTreeRegressor	0.97	1	6.28
DecisionTreeRegressor	0.97	1	6.34
AdaBoostRegressor	0.93	0.9	9.92
BaggingRegressor	0.84	0.9	14.8
RandomForestRegressor	0.82	0.8	15.7
HistGradientBoostingRegressor	0.76	0.8	18.3
LGBMRegressor	0.69	0.7	20.9
KNeighborsRegressor	0.43	0.5	28.2
PoissonRegressor	0.43	0.5	28.3
LarsCV	0.28	0.3	31.7
OrthogonalMatchingPursuitCV	0.28	0.3	31.7
LassoLarsIC	0.28	0.3	31.7
LinearRegression	0.28	0.3	31.7
TransformedTargetRegressor	0.28	0.3	31.7
Lars	0.28	0.3	31.7
LassoLarsCV	0.28	0.3	31.7
LassoCV	0.28	0.3	31.7
SGDRegressor	0.28	0.3	31.7
Ridge	0.28	0.3	31.7
BayesianRidge	0.28	0.3	31.8
ElasticNetCV	0.28	0.3	31.8
Lasso	0.27	0.3	31.9
LassoLars	0.27	0.3	31.9
RidgeCV	0.27	0.3	32
ElasticNet	0.21	0.3	33.2
PassiveAggressiveRegressor	0.21	0.3	33.2
HuberRegressor	0.2	0.3	33.5
GammaRegressor	0.18	0.2	33.8
TweedieRegressor	0.17	0.2	34.2
OrthogonalMatchingPursuit	0.16	0.2	34.3
RANSACRegressor	0.16	0.2	34.3
SVR	0.15	0.2	34.6
NuSVR	0.14	0.2	34.8

LinearSVR	0.11	0.2	35.3
DummyRegressor	-0.08	0	39
QuantileRegressor	-0.15	-0.1	40.2
KernelRidge	-0.54	-0.4	46.4
MLPRegressor	-0.62	-0.5	47.6
GaussianProcessRegressor	-18.4	-17	165

Table S26: ML performance metrics for predicting the density ($kg \cdot m^{-3}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	511 %	19.609	1196.89	34.596	0.181
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	509 %	15.737	532.309	23.072	0.274
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	318 %	15.615	900.169	30.003	0.384
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	315 %	11.742	320.004	17.889	0.564
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	536 %	19.679	1199.26	34.63	0.179
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	533 %	15.793	538.871	23.214	0.265
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	331 %	15.651	899.065	29.984	0.385
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	328 %	11.762	322.08	17.947	0.561
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	282 %	19.696	1371.876	37.039	0.061
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	281 %	16.03	809.423	28.45	-0.104
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	9.255	447.176	21.147	0.694
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	21 %	7.389	219.42	14.813	0.701
======== ExtraTreesRegressor - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	274 %	14.906	926.867	30.444	0.366
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	272 %	11.131	379.549	19.482	0.483
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	7.906	396.085	19.902	0.729
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	35 %	5.938	150.474	12.267	0.795
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	231 %	11.12	797.263	28.236	0.454
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	230 %	7.356	262.715	16.208	0.642
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	22 %	7.144	471.201	21.707	0.678
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	21 %	4.625	148.901	12.203	0.797
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	157 %	12.649	814.031	28.531	0.443
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	155 %	8.765	267.961	16.37	0.635
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	249 %	19.523	1174.883	34.277	0.196
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	247 %	15.77	622.273	24.945	0.152
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	235 %	15.093	624.011	24.98	0.573
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	236 %	14.333	553.323	23.523	0.246
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	194 %	18.248	1231.936	35.099	0.157
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	192 %	14.349	626.229	25.025	0.146
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	386 %	23.635	1532.74	39.15	-0.049
Exp x NIST	3 %	3.988	489.328	22.121	0.665

NIST x Model	386 %	20.061	929.966	30.495	-0.268
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	224 %	16.514	1057.385	32.517	0.277
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	222 %	12.758	432.181	20.789	0.411
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	74 %	11	488.869	22.11	0.665
Exp x NIST	3 %	3.988	489.328	22.121	0.665
NIST x Model	73 %	8.849	224.181	14.973	0.694

S2.7 Volume

Table S27: Evaluation of multiple ML models to the volume ($m^3 \cdot kg^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreesRegressor	1	1	0.01
DecisionTreeRegressor	0.99	1	0.02
XGBRegressor	0.99	1	0.02
GradientBoostingRegressor	0.99	1	0.02
ExtraTreeRegressor	0.99	1	0.02
NuSVR	0.97	1	0.03
BaggingRegressor	0.97	1	0.03
RandomForestRegressor	0.97	1	0.03
AdaBoostRegressor	0.95	1	0.04
SVR	0.86	0.9	0.07
GaussianProcessRegressor	0.69	0.7	0.1
KNeighborsRegressor	0.69	0.7	0.1
MLPRegressor	0.57	0.6	0.12
GammaRegressor	0.17	0.2	0.16
TweedieRegressor	0.12	0.2	0.17
LinearSVR	0	0.1	0.18
HuberRegressor	0	0.1	0.18
RANSACRegressor	-0.01	0.1	0.18
PassiveAggressiveRegressor	-0.04	0	0.18
SGDRegressor	-0.05	0	0.19
PoissonRegressor	-0.08	0	0.19
BayesianRidge	-0.09	-0	0.19
Ridge	-0.11	-0	0.19
RidgeCV	-0.11	-0	0.19
ElasticNetCV	-0.11	-0	0.19
LassoCV	-0.11	-0	0.19
LinearRegression	-0.11	-0	0.19
TransformedTargetRegressor	-0.11	-0	0.19
OrthogonalMatchingPursuitCV	-0.11	-0	0.19
Lars	-0.11	-0	0.19
LarsCV	-0.11	-0	0.19
LassoLarsCV	-0.11	-0	0.19
LassoLarsIC	-0.11	-0	0.19
QuantileRegressor	-0.13	-0	0.19
LGBMRegressor	-0.19	-0.1	0.2
HistGradientBoostingRegressor	-0.21	-0.1	0.2

DummyRegressor	-0.32	-0.2	0.21
ElasticNet	-0.32	-0.2	0.21
LassoLars	-0.32	-0.2	0.21
Lasso	-0.32	-0.2	0.21
OrthogonalMatchingPursuit	-0.46	-0.3	0.22
KernelRidge	-0.54	-0.4	0.23

Table S28: ML performance metrics for predicting the volume ($m^3 \cdot kg^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	348 %	0.249	0.228	0.478	-0.366
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	334 %	0.249	0.228	0.478	-0.366
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	290 %	0.205	0.149	0.386	0.11
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	277 %	0.205	0.149	0.386	0.11
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	917 %	0.322	0.244	0.494	-0.458
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	784 %	0.322	0.243	0.493	-0.455
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	689 %	0.222	0.096	0.31	0.426
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	588 %	0.222	0.095	0.309	0.429
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	281 %	0.214	0.207	0.455	-0.239
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	264 %	0.213	0.207	0.455	-0.24
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	255 %	0.188	0.151	0.389	0.095
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	240 %	0.188	0.151	0.389	0.095
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	819 %	0.302	0.23	0.48	-0.377
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	701 %	0.302	0.23	0.479	-0.374
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	646 %	0.219	0.099	0.315	0.406
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	552 %	0.218	0.099	0.314	0.408
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	34 %	0.111	0.172	0.415	-0.032
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	26 %	0.111	0.173	0.415	-0.032
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	0.015	0.002	0.047	0.987
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	11 %	0.015	0.002	0.047	0.987
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	0.113	0.175	0.418	-0.045
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	21 %	0.111	0.175	0.418	-0.045
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	0.008	0.001	0.034	0.993
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	8 %	0.007	0.001	0.032	0.994
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	35 %	0.114	0.184	0.429	-0.1
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	26 %	0.114	0.184	0.429	-0.1
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	25 %	0.022	0.004	0.063	0.976
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	18 %	0.021	0.004	0.063	0.976
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	442 %	0.227	0.193	0.439	-0.153
Exp x NIST	12 %	0.001	0	0.009	0.999

NIST x Model	377 %	0.226	0.192	0.438	-0.15
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	933 %	0.343	0.221	0.47	-0.324
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	872 %	0.341	0.221	0.47	-0.32
======== NuSVR_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	118 %	0.146	0.159	0.399	0.047
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	111 %	0.145	0.159	0.399	0.048
======== NuSVR_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	60 %	0.115	0.17	0.412	-0.017
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	49 %	0.115	0.17	0.412	-0.018
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	30 %	0.111	0.175	0.418	-0.047
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	21 %	0.11	0.175	0.418	-0.048
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	0.013	0.002	0.046	0.987
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	8 %	0.012	0.002	0.046	0.987
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	193 %	0.149	0.193	0.439	-0.154
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	101 %	0.148	0.191	0.437	-0.143
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	170 %	0.061	0.028	0.167	0.833
Exp x NIST	12 %	0.001	0	0.009	0.999
NIST x Model	82 %	0.06	0.026	0.161	0.845

S2.8 Enthalpy

Table S29: Evaluation of multiple ML models for the enthalpy (kJ·mol^{-1}) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in kJ·mol^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
XGBRegressor	0.9	0.9	0.79
ExtraTreeRegressor	0.9	0.9	0.81
GradientBoostingRegressor	0.9	0.9	0.81
ExtraTreesRegressor	0.9	0.9	0.83
RandomForestRegressor	0.89	0.9	0.84
BaggingRegressor	0.89	0.9	0.84
DecisionTreeRegressor	0.89	0.9	0.85
KNeighborsRegressor	0.88	0.9	0.88
AdaBoostRegressor	0.85	0.9	0.99
HistGradientBoostingRegressor	0.62	0.6	1.58
LGBMRegressor	0.62	0.6	1.58
SVR	0.54	0.6	1.74
NuSVR	0.52	0.5	1.78
ElasticNetCV	0.08	0.1	2.46
RidgeCV	0.08	0.1	2.46
BayesianRidge	0.08	0.1	2.46
LassoCV	0.08	0.1	2.46
SGDRegressor	0.08	0.1	2.46
Ridge	0.08	0.1	2.46
LinearRegression	0.08	0.1	2.46
TransformedTargetRegressor	0.08	0.1	2.46
OrthogonalMatchingPursuitCV	0.08	0.1	2.46
LassoLarsCV	0.08	0.1	2.46
LassoLarsIC	0.08	0.1	2.46
LarsCV	0.08	0.1	2.46
Lars	0.08	0.1	2.46
PoissonRegressor	0.06	0.1	2.48
TweedieRegressor	0.05	0.1	2.49
GammaRegressor	0.05	0.1	2.5
PassiveAggressiveRegressor	0.02	0.1	2.53
OrthogonalMatchingPursuit	0.02	0.1	2.54
ElasticNet	0	0	2.56
DummyRegressor	-0.03	0	2.6
LassoLars	-0.03	0	2.6
Lasso	-0.03	0	2.6
QuantileRegressor	-0.04	-0	2.61

LinearSVR	-0.09	-0.1	2.67
HuberRegressor	-0.09	-0.1	2.68
RANSACRegressor	-0.1	-0.1	2.68
MLPRegressor	-0.46	-0.4	3.1
KernelRidge	-19.1	-19	11.5
GaussianProcessRegressor	-102	-99	26

Table S30: ML performance metrics for predicting enthalpy ($kJ \cdot mol^{-1}$) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $kJ \cdot mol^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	97 %	1.616	10.357	3.218	-1.077
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	14 %	1.231	3.067	1.751	-0.109
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	66 %	1.196	4.801	2.191	0.037
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	12 %	0.954	1.581	1.257	0.428
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	78 %	1.156	6.168	2.484	-0.237
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.746	0.986	0.993	0.644
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	64 %	1.028	4.344	2.084	0.129
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	10 %	0.788	1.067	1.033	0.614
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	78 %	1.158	6.027	2.455	-0.209
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	10 %	0.775	1.038	1.019	0.625
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	67 %	1.035	4.627	2.151	0.072
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.753	1.019	1.009	0.632
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	76 %	1.008	5.73	2.394	-0.149
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	8 %	0.626	0.743	0.862	0.731
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	66 %	0.885	4.345	2.084	0.129
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.646	0.777	0.882	0.719
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	63 %	0.542	3.83	1.957	0.232
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	7 %	0.587	0.599	0.774	0.784
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.253	0.892	0.945	0.821
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.817	4.384	2.094	-0.585
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	63 %	0.639	4.259	2.064	0.146
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	8 %	0.605	0.743	0.862	0.731
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	0.171	0.476	0.69	0.905
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.793	4.341	2.084	-0.569
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	65 %	0.746	5.103	2.259	-0.023
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.725	1.595	1.263	0.424
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	0.14	0.821	0.906	0.835
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.81	4.328	2.08	-0.565
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	62 %	0.49	3.935	1.984	0.211
Exp x NIST	71 %	0.841	4.688	2.165	0.06

NIST x Model	8 %	0.642	0.679	0.824	0.755
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.254	0.957	0.978	0.808
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.833	4.366	2.09	-0.579
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	90 %	2.561	19.217	4.384	-2.853
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	22 %	2.21	13.358	3.655	-3.829
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	61 %	1.558	6.07	2.464	-0.217
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	16 %	1.403	3.727	1.931	-0.347
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	64 %	0.68	4.244	2.06	0.149
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.684	0.828	0.91	0.701
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.193	0.839	0.916	0.832
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.778	4.085	2.021	-0.477
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	63 %	0.649	3.921	1.98	0.214
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	7 %	0.53	0.576	0.759	0.792
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.266	0.838	0.915	0.832
Exp x NIST	71 %	0.841	4.688	2.165	0.06
NIST x Model	9 %	0.8	4.194	2.048	-0.516

S2.9 Viscosity

Table S31: Evaluation of multiple ML models to the viscosity (µPa·s) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in µPa·s are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreesRegressor	0.99	1	0.23
DecisionTreeRegressor	0.99	1	0.24
XGBRegressor	0.99	1	0.26
ExtraTreeRegressor	0.99	1	0.26
GradientBoostingRegressor	0.98	1	0.29
NuSVR	0.9	0.9	0.67
SVR	0.89	0.9	0.69
LinearSVR	0.75	0.8	1.06
HuberRegressor	0.75	0.8	1.06
RANSACRegressor	0.74	0.8	1.08
PassiveAggressiveRegressor	0.71	0.7	1.15
BaggingRegressor	0.61	0.6	1.32
AdaBoostRegressor	0.6	0.6	1.35
GaussianProcessRegressor	0.52	0.5	1.48
QuantileRegressor	-0.04	-0	2.17
DummyRegressor	-0.3	-0.3	2.42
LassoLarsCV	-0.3	-0.3	2.42
ElasticNetCV	-0.3	-0.3	2.42
LassoCV	-0.3	-0.3	2.42
LassoLars	-0.3	-0.3	2.42
Lasso	-0.3	-0.3	2.42
LassoLarsIC	-0.3	-0.3	2.42
LarsCV	-0.3	-0.3	2.42
ElasticNet	-0.3	-0.3	2.42
BayesianRidge	-0.3	-0.3	2.42
RandomForestRegressor	-0.38	-0.3	2.5
OrthogonalMatchingPursuitCV	-0.39	-0.3	2.5
OrthogonalMatchingPursuit	-0.39	-0.3	2.5
GammaRegressor	-0.43	-0.4	2.54
TweedieRegressor	-0.48	-0.4	2.59
PoissonRegressor	-0.76	-0.7	2.82
RidgeCV	-0.78	-0.7	2.83
Ridge	-0.81	-0.8	2.86
Lars	-0.81	-0.8	2.86
LinearRegression	-0.81	-0.8	2.86
TransformedTargetRegressor	-0.81	-0.8	2.86

SGDRegressor	-0.91	-0.9	2.94
HistGradientBoostingRegressor	-1.16	-1.1	3.13
LGBMRegressor	-1.48	-1.4	3.35
MLPRegressor	-1.77	-1.7	3.53
KNeighborsRegressor	-4.03	-3.9	4.77
KernelRidge	-32.5	-31	12.3

Table S32: ML performance metrics for predicting viscosity (µPa·s) in the vapor phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in µPa·s are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	1.912	83.853	9.157	-0.092
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	9 %	1.153	8.034	2.834	0.172
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	1.758	77.686	8.814	-0.011
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	10 %	1.164	7.347	2.711	0.243
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	1.92	84.556	9.195	-0.101
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	8 %	1.143	8.155	2.856	0.16
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	1.755	77.308	8.792	-0.006
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	10 %	1.174	7.479	2.735	0.23
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	2.779	83.357	9.13	-0.085
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	18 %	2.152	12.037	3.469	-0.24
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	2.561	78.663	8.869	-0.024
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	18 %	2.035	10.228	3.198	-0.054
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	2.804	83.471	9.136	-0.087
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	18 %	2.176	12.161	3.487	-0.253
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	2.568	78.632	8.867	-0.024
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	18 %	2.049	10.349	3.217	-0.066
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	1.461	81.98	9.054	-0.067
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	6 %	0.692	7.724	2.779	0.204
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	1.041	72.218	8.498	0.06
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	7 %	0.63	11.976	3.461	-0.234
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.311	80.682	8.982	-0.05
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	4 %	0.545	6.48	2.546	0.332
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.622	36.495	6.041	0.525
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	12 %	0.752	40.426	6.358	-3.164
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	1.418	81.386	9.021	-0.06
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	5 %	0.657	7.322	2.706	0.246
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.878	57.722	7.597	0.249
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	8 %	0.516	10.028	3.167	-0.033
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	1.733	79.753	8.93	-0.038
Exp x NIST	2 %	0.87	78.004	8.832	-0.016

NIST x Model	9 %	1.065	8.385	2.896	0.136
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	29 %	4.439	118.805	10.9	-0.547
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	27 %	3.616	40.775	6.386	-3.2
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	2.663	78.612	8.866	-0.023
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	19 %	2.146	11.986	3.462	-0.235
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	1.377	80.471	8.971	-0.048
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	5 %	0.628	6.84	2.615	0.295
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.979	46.56	6.824	0.394
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	15 %	1.031	46.327	6.806	-3.772
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	1.801	80.574	8.976	-0.049
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	9 %	1.09	7.704	2.776	0.206
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	1.499	59.811	7.734	0.221
Exp x NIST	2 %	0.87	78.004	8.832	-0.016
NIST x Model	16 %	1.267	23.936	4.892	-1.466

S3. Supercritical Phase

S3.1 Best metrics

On Table S33, the units of MAE and RMSE are reported in the same units as the target property, while MSE carries squared units. For instance, when predicting density ($kg \cdot m^{-3}$) or sound speed ($m \cdot s^{-1}$), MAE and RMSE are expressed in $kg \cdot m^{-3}$ and $m \cdot s^{-1}$, respectively, while MSE carries squared units, such as $(kg \cdot m^{-3})^2$ or $(m \cdot s^{-1})^2$. The MAPE, in contrast, is unitless and expressed as a percentage. The R^2 metric is also unitless

Tables even-numbered from Table 35 to Table S30 presents all the ML performance metrics for predicting the corresponding investigated property in supercritical phase. Data in red represents the best model for each property.

Table S33: ML performance metrics for best-performing models for predicting various thermophysical properties in the supercritical phase, including density ($kg \cdot m^{-3}$), volume ($m^3 \cdot kg^{-1}$), enthalpy ($kJ \cdot mol^{-1}$), $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$), $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$), sound speed ($m \cdot s^{-1}$), Joule-Thomson Coefficient ($K \cdot MPa^{-1}$), and viscosity ($\mu Pa \cdot s$). The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in the respective property units are presented.

Cp – Gradient Boosting – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	6 %	7.542	863.444	29.384	0.818
Exp x NIST	4 %	2.389	32.386	5.691	0.993
NIST x Model	8 %	8.93	1004.632	31.696	0.782
Cv – ExtraTrees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	1 %	0.385	1.775	1.332	0.748
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.55	0.819	0.905	0.813
Joule-Thomson – XGB – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	3.0%	0.130	0.057	0.238	0.979
Exp x NIST	9.0%	0.444	0.581	0.762	0.787
NIST x Model	10.0%	0.407	0.497	0.705	0.576
Sound Speed – Gradient Boosting – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	**R^2**
Exp x Model	47 %	16.152	1399.825	37.414	0.999
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	2 %	14.617	471.024	21.703	0.9999

Density – Extra Trees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	4 %	5.06	153.119	12.374	0.982
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	3 %	3.93	48.208	6.943	0.994
Volume – Extra Trees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	4.0%	0.000	0.000	0.001	0.971
Exp x NIST	1.0%	0.000	0.000	0.001	0.983
NIST x Model	3.0%	0.000	0.000	0.001	0.988
Enthalpy –XGB – CV = 10					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	47 %	1.034	4.05	2.012	0.637
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	12 %	1.381	8.699	2.949	-0.296
Viscosity – Extra Trees – CV = LOO					
Comparison	**MAPE**	**MAE**	**MSE**	**RMSE**	R^2
Exp x Model	4 %	0.796	6.485	2.547	0.962
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	6 %	2.383	74.552	8.634	0.644

S3.2 Isobaric heat capacity (Cp)

Table S34: Evaluation of multiple ML models for $\boldsymbol{Cp}$ in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in J·mol^{-1}·K^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
XGBRegressor	0.68	0.70	12.52
KNeighborsRegressor	0.64	0.67	13.14
ExtraTreesRegressor	0.63	0.65	13.37
HuberRegressor	0.61	0.64	13.64
PassiveAggressiveRegressor	0.55	0.58	14.76
SVR	0.52	0.55	15.25
NuSVR	0.44	0.48	16.44
LinearSVR	0.33	0.38	17.97
RANSACRegressor	0.31	0.36	18.23
GammaRegressor	0.31	0.36	18.23
RandomForestRegressor	0.29	0.34	18.54
GradientBoostingRegressor	0.09	0.15	20.92
ElasticNet	0.00	0.07	21.95
AdaBoostRegressor	-0.00	0.06	22.02
TweedieRegressor	-0.01	0.06	22.04
BaggingRegressor	-0.06	0.01	22.58
PoissonRegressor	-0.14	-0.07	23.47
OrthogonalMatchingPursuit	-0.21	-0.13	24.13
ExtraTreeRegressor	-0.25	-0.17	24.54
DecisionTreeRegressor	-0.29	-0.20	24.90
RidgeCV	-0.38	-0.29	25.85
BayesianRidge	-0.44	-0.35	26.37
Lasso	-0.46	-0.37	26.57
LassoLars	-0.46	-0.37	26.57
ElasticNetCV	-0.48	-0.38	26.75
Ridge	-0.56	-0.45	27.41
SGDRegressor	-0.57	-0.47	27.55
LassoCV	-0.57	-0.47	27.57
LinearRegression	-0.58	-0.48	27.61
TransformedTargetRegressor	-0.58	-0.48	27.61
OrthogonalMatchingPursuitCV	-0.58	-0.48	27.61
LassoLarsIC	-0.58	-0.48	27.61
LassoLarsCV	-0.58	-0.48	27.61
LarsCV	-0.58	-0.48	27.61
Lars	-0.58	-0.48	27.61
DummyRegressor	-0.98	-0.84	30.87

HistGradientBoostingRegressor	-1.50	-1.33	34.70
LGBMRegressor	-1.64	-1.46	35.70
MLPRegressor	-5.27	-4.85	54.99
KernelRidge	-10.18	-9.44	73.45
GaussianProcessRegressor	-266.51	-248.68	359.27

Table S35: ML performance metrics for predicting $\boldsymbol{Cp}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	63 %	39.72	5023	70.87	-0.057
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	62 %	39.83	5056	71.1	-0.099
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	49 %	33.81	3820	61.81	0.196
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	48 %	33.89	3813	61.75	0.171
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	64 %	39.83	5033	70.94	-0.059
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	62 %	39.96	5066	71.17	-0.101
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	52 %	35.34	3855	62.09	0.189
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	52 %	35.46	3862	62.14	0.161
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	55 %	36.4	4552	67.47	0.042
Exp x NIST	4 %	2.389	32.39	5.691	0.993

NIST x Model	53 %	36.37	4549	67.44	0.012
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43 %	31.58	3827	61.86	0.195
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	43 %	31.66	3806	61.69	0.173
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	55 %	36.49	4559	67.52	0.041
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	53 %	36.47	4556	67.5	0.01
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	44 %	31.66	3828	61.87	0.195
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	44 %	31.73	3807	61.7	0.173
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	17.4	2449	49.49	0.485
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	16 %	17.81	2464	49.64	0.465
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	11.49	1226	35.01	0.742
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	11 %	12.54	1310	36.2	0.715
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	12.92	1936	44	0.593
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	11 %	13.46	1988	44.59	0.568
======== ExtraTreesRegressor - CV = LOO ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	7.605	841	29	0.823
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	8 %	8.979	1019	31.92	0.779
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	15.82	2273	47.68	0.522
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	14 %	16.23	2309	48.05	0.498
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	7.542	863.4	29.38	0.818
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	8 %	8.93	1005	31.7	0.782
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	21.5	2984	54.63	0.372
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	21 %	21.5	2990	54.68	0.35
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	13.23	819.5	28.63	0.828
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	16 %	14.48	927.6	30.46	0.798
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	33.89	4679	68.41	0.015
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	42 %	32.6	4529	67.3	0.016
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43 %	34.49	5110	71.48	-0.075

Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	40 %	33.55	4976	70.54	-0.081
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	16.33	2468	49.68	0.481
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	13 %	16.37	2461	49.61	0.465
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	9.494	927.6	30.46	0.805
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	9 %	10.57	1050	32.4	0.772
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	27 %	26.27	3723	61.02	0.217
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	28 %	26.33	3670	60.58	0.202
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23 %	22.15	2219	47.1	0.533
Exp x NIST	4 %	2.389	32.39	5.691	0.993
NIST x Model	25 %	22.94	2248	47.41	0.512

S3.3 Isochoric heat capacity (Cv)

Table S36: Evaluation of multiple ML models for $\boldsymbol{Cv}$ in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
KNeighborsRegressor	0.98	0.98	0.23
ExtraTreesRegressor	0.97	0.98	0.28
RandomForestRegressor	0.97	0.97	0.32
BaggingRegressor	0.96	0.96	0.36
HistGradientBoostingRegressor	0.95	0.96	0.37
LGBMRegressor	0.94	0.95	0.41
AdaBoostRegressor	0.93	0.93	0.47
GradientBoostingRegressor	0.92	0.92	0.49
XGBRegressor	0.91	0.91	0.53
ExtraTreeRegressor	0.90	0.90	0.55
DecisionTreeRegressor	0.88	0.88	0.60
NuSVR	0.73	0.75	0.90
SVR	0.73	0.74	0.90
HuberRegressor	0.26	0.30	1.49
GammaRegressor	0.21	0.25	1.54
TweedieRegressor	0.20	0.24	1.55
PoissonRegressor	0.19	0.23	1.56
OrthogonalMatchingPursuit	0.18	0.22	1.57
ElasticNet	0.17	0.22	1.57
ElasticNetCV	0.17	0.21	1.58
LassoCV	0.17	0.21	1.58
RidgeCV	0.17	0.21	1.58
BayesianRidge	0.17	0.21	1.58
SGDRegressor	0.16	0.21	1.58
Ridge	0.16	0.20	1.59
LinearRegression	0.16	0.20	1.59
TransformedTargetRegressor	0.16	0.20	1.59
LassoLarsCV	0.16	0.20	1.59
LassoLarsIC	0.16	0.20	1.59
LarsCV	0.16	0.20	1.59
Lars	0.16	0.20	1.59
OrthogonalMatchingPursuitCV	0.16	0.20	1.59
LinearSVR	0.13	0.17	1.62
Lasso	0.09	0.14	1.65
LassoLars	0.09	0.14	1.65
PassiveAggressiveRegressor	0.04	0.08	1.70

DummyRegressor	-0.15	-0.10	1.86
RANSACRegressor	-0.26	-0.19	1.94
GaussianProcessRegressor	-5.59	-5.26	4.44
MLPRegressor	-176.14	-167.29	23.05
KernelRidge	-317.41	-301.49	30.90

Table S37: ML performance metrics for predicting $\boldsymbol{Cv}$ ($J \cdot mol^{-1} \cdot K^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $J \cdot mol^{-1} \cdot K^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.532	5.844	2.418	0.17
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	5 %	1.506	3.844	1.961	0.122
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	1.452	5.118	2.262	0.273
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	5 %	1.448	3.362	1.833	0.232
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.568	5.836	2.416	0.171
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	5 %	1.539	3.884	1.971	0.113
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	1.456	5.175	2.275	0.265
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	5 %	1.464	3.443	1.856	0.214
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.508	2.718	1.649	0.614
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.609	1.363	1.168	0.689
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.385	1.775	1.332	0.748
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.55	0.819	0.905	0.813
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	2 %	0.547	2.877	1.696	0.591
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.595	1.428	1.195	0.674
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.424	2.601	1.613	0.631
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.535	1.463	1.21	0.666
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.647	3.101	1.761	0.56
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.697	1.706	1.306	0.611
======== KNeighbors ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.495	2.594	1.611	0.632
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.668	1.501	1.225	0.657
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.67	3.116	1.765	0.558
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.712	1.666	1.291	0.62
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	1.895	8.291	2.879	-0.177
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	6 %	1.776	5.446	2.334	-0.243
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	2.772	12.044	3.47	-0.71
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	9 %	2.689	11.112	3.333	-1.537
======== RandomForest ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	1 %	0.472	2.057	1.434	0.708
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.564	0.987	0.994	0.775
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.816	3.771	1.942	0.465
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	3 %	0.8	2.138	1.462	0.512

======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	2 %	0.694	2.796	1.672	0.603
Exp x NIST	1 %	0.483	1	1	0.858
NIST x Model	2 %	0.664	1.484	1.218	0.661

S3.4 Joule-Thomson

Table S38: Evaluation of multiple ML models for the Joule-Thomson coefficient ($K \cdot MPa^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $K \cdot MPa^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
GradientBoostingRegressor	0.99	1	0.12
XGBRegressor	0.99	0.99	0.14
DecisionTreeRegressor	0.98	0.99	0.2
AdaBoostRegressor	0.98	0.99	0.23
BaggingRegressor	0.98	0.98	0.24
RandomForestRegressor	0.98	0.98	0.24
ExtraTreesRegressor	0.96	0.97	0.3
OrthogonalMatchingPursuit	0.77	0.84	0.75
LarsCV	0.72	0.8	0.84
LassoLarsIC	0.72	0.8	0.84
Lars	0.72	0.8	0.84
LassoLarsCV	0.72	0.8	0.84
OrthogonalMatchingPursuitCV	0.72	0.8	0.84
LinearRegression	0.72	0.8	0.84
TransformedTargetRegressor	0.72	0.8	0.84
LassoCV	0.72	0.8	0.84
BayesianRidge	0.71	0.79	0.86
ElasticNetCV	0.7	0.79	0.87
KNeighborsRegressor	0.7	0.79	0.87
RidgeCV	0.7	0.78	0.87
Ridge	0.7	0.78	0.87
MLPRegressor	0.66	0.76	0.92
SGDRegressor	0.64	0.74	0.95
PoissonRegressor	0.6	0.71	1.01
NuSVR	0.58	0.7	1.02
SVR	0.58	0.7	1.03
HuberRegressor	0.57	0.69	1.04
ExtraTreeRegressor	0.54	0.67	1.07
TweedieRegressor	0.25	0.47	1.37
LinearSVR	0.25	0.47	1.37
ElasticNet	0.24	0.46	1.38
GammaRegressor	0.17	0.4	1.45
GaussianProcessRegressor	0.15	0.39	1.46
RANSACRegressor	0.11	0.37	1.49
Lasso	0.05	0.32	1.54

LassoLars	0.05	0.32	1.54
LGBMRegressor	-0.54	-0.1	1.96
DummyRegressor	-0.54	-0.1	1.96
HistGradientBoostingRegressor	-0.54	-0.1	1.96
PassiveAggressiveRegressor	-0.59	-0.14	2
QuantileRegressor	-0.75	-0.25	2.1
KernelRidge	-5.84	-3.89	4.14

Table S39: ML performance metrics for predicting the Joule-Thomson coefficient ($K \cdot MPa^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $K \cdot MPa^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	23 %	0.715	0.823	0.907	0.698
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	22 %	0.655	0.608	0.78	0.481
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	0.585	0.501	0.708	0.816
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	18 %	0.584	0.44	0.664	0.624
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	0.669	0.719	0.848	0.736
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	22 %	0.669	0.604	0.777	0.485
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	17 %	0.568	0.44	0.664	0.838
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	20 %	0.669	0.553	0.744	0.528
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	24 %	0.778	0.914	0.956	0.664
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	23 %	0.642	0.601	0.775	0.488
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	19 %	0.628	0.571	0.755	0.79
Exp x NIST	9 %	0.444	0.581	0.762	0.787

NIST x Model	18 %	0.545	0.394	0.628	0.664
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	24 %	0.756	0.847	0.92	0.689
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	23 %	0.644	0.569	0.754	0.515
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	0.603	0.509	0.713	0.813
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	18 %	0.57	0.388	0.623	0.669
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	0.302	0.112	0.335	0.959
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	16 %	0.58	0.547	0.739	0.534
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0.197	0.056	0.237	0.979
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	12 %	0.497	0.575	0.758	0.509
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	7 %	0.256	0.118	0.343	0.957
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	14 %	0.527	0.534	0.731	0.544
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.112	0.02	0.14	0.993
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	11 %	0.447	0.537	0.733	0.542
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.364	0.216	0.465	0.92
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	14 %	0.504	0.383	0.619	0.673
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.13	0.057	0.238	0.979
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	10 %	0.407	0.497	0.705	0.576
======== NeuralNetwork - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	54 %	1.991	6.125	2.475	-1.251
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	51 %	1.603	3.518	1.876	-2.001
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	56 %	1.886	5.724	2.393	-1.104
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	54 %	1.582	3.794	1.948	-2.236
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	0.47	0.37	0.608	0.864
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	15 %	0.55	0.534	0.731	0.544
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.119	0.027	0.165	0.99
Exp x NIST	9 %	0.444	0.581	0.762	0.787
NIST x Model	10 %	0.419	0.476	0.69	0.594

S3.5 Sound Speed

Table S40: Evaluation of multiple ML models for the Sound Speed ($m \cdot s^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreeRegressor	1	1	34
ExtraTreesRegressor	1	1	42.3
RandomForestRegressor	1	1	44.8
BaggingRegressor	1	1	46.4
GaussianProcessRegressor	1	1	46.6
GradientBoostingRegressor	1	1	50.7
XGBRegressor	1	1	61
DecisionTreeRegressor	0.99	0.99	79.3
AdaBoostRegressor	0.99	0.99	89
LGBMRegressor	0.99	0.99	89.8
KNeighborsRegressor	0.99	0.99	92.2
HistGradientBoostingRegressor	0.99	0.99	92.6
RidgeCV	0.91	0.91	308
Ridge	0.91	0.91	308
SGDRegressor	0.91	0.91	308
BayesianRidge	0.91	0.91	309
LassoLars	0.91	0.91	309
Lasso	0.91	0.91	309
LassoCV	0.91	0.91	309
LarsCV	0.91	0.91	309
Lars	0.91	0.91	309
LassoLarsIC	0.91	0.91	309
OrthogonalMatchingPursuitCV	0.91	0.91	309
LassoLarsCV	0.91	0.91	309
LinearRegression	0.91	0.91	309
TransformedTargetRegressor	0.91	0.91	309
OrthogonalMatchingPursuit	0.91	0.91	311
HuberRegressor	0.9	0.9	323
PassiveAggressiveRegressor	0.9	0.9	325
ElasticNet	0.83	0.84	418
RANSACRegressor	0.81	0.82	447
ElasticNetCV	0.72	0.73	545
TweedieRegressor	0.71	0.72	555
GammaRegressor	0.69	0.7	571
PoissonRegressor	0.66	0.67	597
NuSVR	-0.04	0	1045

DummyRegressor	-0.05	0	1049
KernelRidge	-0.24	-0.19	1140
SVR	-0.34	-0.27	1183
LinearSVR	-0.89	-0.81	1408
MLPRegressor	-1.22	-1.12	1524

Table S41: ML performance metrics for predicting the sound speed ($m \cdot s^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m \cdot s^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	100 %	276.601	122516.2	350.023	0.88
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	44 %	273.649	120471.1	347.089	0.881
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	89 %	240.288	95934.21	309.732	0.906
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	35 %	237.383	94017.49	306.623	0.907
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	100 %	276.756	122700.6	350.286	0.879
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	44 %	273.803	120650	347.347	0.881
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	89 %	240.338	95911.67	309.696	0.906
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	35 %	237.42	93994.86	306.586	0.907
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	93 %	271.686	129598.6	359.998	0.873
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	39 %	268.731	127654.6	357.288	0.874
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	86 %	234.72	94461.36	307.346	0.907
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	33 %	231.797	92618.5	304.333	0.908
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2

Exp x Model	93 %	271.693	129602.1	360.003	0.873
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	39 %	268.738	127658.2	357.293	0.874
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	86 %	234.721	94461.5	307.346	0.907
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	33 %	231.798	92618.7	304.333	0.908
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	42.816	4126.944	64.241	0.996
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	5 %	40.96	3358.524	57.953	0.997
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	48 %	31.328	3259.52	57.092	0.997
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	3 %	29.303	2328.889	48.259	0.998
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	48 %	33.402	3973.952	63.039	0.996
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	4 %	31.368	3092.081	55.606	0.997
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	19.585	1647.562	40.59	0.998
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	2 %	17.738	710.822	26.661	0.999
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	39.249	3485.827	59.041	0.997
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	6 %	38.12	2747.727	52.419	0.997
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	16.152	1399.825	37.414	0.999
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	2 %	14.617	471.024	21.703	0.9999
======== HistGradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	52 %	64.68	11432.47	106.923	0.989
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	6 %	62.677	10572.67	102.823	0.99

======== HistGradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	49 %	31.101	3356.128	57.932	0.997
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	4 %	29.5	2439.752	49.394	0.998
======== LGBM_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	50 %	72.011	13536.84	116.348	0.987
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	8 %	70.269	12819.22	113.222	0.987
======== LGBM_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	49 %	37.222	3872.772	62.232	0.996
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	4 %	35.568	2969.646	54.494	0.997
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	57 %	155.561	54204.19	232.818	0.947
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	13 %	152.996	53229.26	230.715	0.947
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	58 %	111.901	29691.15	172.311	0.971
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	10 %	109.695	28547.96	168.961	0.972
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	46.224	5845.148	76.454	0.994
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	6 %	44.762	5089.931	71.344	0.995
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	48 %	25.35	2314.107	48.105	0.998
Exp x NIST	45 %	3.993	971.914	31.176	0.999
NIST x Model	3 %	24.182	1399.375	37.408	0.999

S3.6 Density

Table S42: Evaluation of multiple ML models for the Density ($kg \cdot m^{-3}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreesRegressor	0.98	0.98	13.9
KNeighborsRegressor	0.97	0.97	15.6
HistGradientBoostingRegressor	0.97	0.97	15.8
RandomForestRegressor	0.97	0.97	15.9
LGBMRegressor	0.97	0.97	16.1
XGBRegressor	0.97	0.97	16.3
BaggingRegressor	0.97	0.97	16.9
GradientBoostingRegressor	0.96	0.97	17.2
DecisionTreeRegressor	0.96	0.96	19.4
ExtraTreeRegressor	0.95	0.96	19.5
AdaBoostRegressor	0.86	0.86	34
ElasticNetCV	0.76	0.77	44.4
Lasso	0.74	0.75	46.2
LassoLars	0.74	0.75	46.2
LassoCV	0.74	0.74	46.6
RidgeCV	0.74	0.74	46.8
Ridge	0.74	0.74	46.8
BayesianRidge	0.74	0.74	46.8
OrthogonalMatchingPursuitCV	0.74	0.74	46.9
LassoLarsIC	0.74	0.74	46.9
LarsCV	0.74	0.74	46.9
LassoLarsCV	0.74	0.74	46.9
Lars	0.74	0.74	46.9
TransformedTargetRegressor	0.74	0.74	46.9
LinearRegression	0.74	0.74	46.9
SGDRegressor	0.74	0.74	47
ElasticNet	0.73	0.73	47.8
LinearSVR	0.71	0.72	49
HuberRegressor	0.68	0.68	51.6
RANSACRegressor	0.66	0.66	53.3
TweedieRegressor	0.61	0.61	57.1
PassiveAggressiveRegressor	0.6	0.61	57.5
GammaRegressor	0.59	0.59	58.7
PoissonRegressor	0.49	0.5	65.3
SVR	0.47	0.48	66.4
OrthogonalMatchingPursuit	0.47	0.47	66.7

NuSVR	0.39	0.39	71.6
DummyRegressor	-0.05	-0.04	93.7
QuantileRegressor	-0.1	-0.08	95.6
MLPRegressor	-1.54	-1.5	145
KernelRidge	-3.58	-3.52	195
GaussianProcessRegressor	-729.6	-719.6	2468

Table S43: ML performance metrics for predicting the density ($kg \cdot m^{-3}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $kg \cdot m^{-3}$ are presented.

======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33 %	43.056	2768.855	52.62	0.668
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	33 %	42.72	2704.024	52	0.673
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	30 %	37.754	2141.908	46.281	0.743
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	30 %	37.428	2078.899	45.595	0.749
======== BaggingRegressorRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33 %	43.058	2770.101	52.632	0.667
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	33 %	42.722	2705.255	52.012	0.673
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	30 %	37.751	2141.948	46.281	0.743
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	30 %	37.426	2078.924	45.595	0.749
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	13 %	17.072	810.173	28.464	0.903
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	12 %	16.105	700.485	26.467	0.915
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	12.389	363.744	19.072	0.956
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	8 %	11.599	263.147	16.222	0.968
======== ExtraTreesRegressor - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	7.533	232.768	15.257	0.972
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	5 %	6.41	132.162	11.496	0.984
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	5.06	153.119	12.374	0.982
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	3 %	3.93	48.208	6.943	0.994
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	11.047	308.107	17.553	0.963
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	7 %	10.097	209.59	14.477	0.975
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	6.731	172.391	13.13	0.979
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	4 %	5.748	69.47	8.335	0.992
======== HistGradientBoosting ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	11.307	334.351	18.285	0.96
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	8 %	10.418	226.994	15.066	0.973
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	15.084	642.315	25.344	0.923
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	11 %	14.246	557.108	23.603	0.933
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	7.991	211.723	14.551	0.975
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	5 %	6.97	111.114	10.541	0.987
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	12 %	17.623	623.259	24.965	0.925
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	11 %	16.695	509.043	22.562	0.939
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	14.777	459.872	21.445	0.945
Exp x NIST	1 %	1.813	106.597	10.325	0.987

NIST x Model	10 %	13.924	359.564	18.962	0.957
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20 %	25.502	1022.624	31.978	0.877
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	20 %	24.93	943.812	30.722	0.886
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	16 %	19.853	683.946	26.152	0.918
Exp x NIST	1 %	1.813	106.597	10.325	0.987
NIST x Model	16 %	19.169	611.536	24.729	0.926

S3.7 Volume

Table S44: Evaluation of multiple ML models for the volume ($m^3 \cdot kg^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

Model	R^2_{adj}	R^2	RMSE
ExtraTreesRegressor	0.98	0.98	0
NuSVR	0.97	0.97	0
XGBRegressor	0.97	0.97	0
GradientBoostingRegressor	0.97	0.97	0
RandomForestRegressor	0.97	0.97	0
BaggingRegressor	0.97	0.97	0
ExtraTreeRegressor	0.96	0.97	0
LGBMRegressor	0.95	0.95	0
HistGradientBoostingRegressor	0.95	0.95	0
DecisionTreeRegressor	0.94	0.94	0
KNeighborsRegressor	0.9	0.9	0
AdaBoostRegressor	0.84	0.84	0
LarsCV	0.46	0.47	0
OrthogonalMatchingPursuitCV	0.46	0.47	0
LassoLarsIC	0.46	0.47	0
LinearRegression	0.46	0.47	0
TransformedTargetRegressor	0.46	0.47	0
Lars	0.46	0.47	0
LassoLarsCV	0.46	0.47	0
Ridge	0.46	0.47	0
BayesianRidge	0.46	0.47	0
LassoCV	0.46	0.47	0
ElasticNetCV	0.46	0.47	0
RidgeCV	0.46	0.47	0
SGDRegressor	0.46	0.47	0
LinearSVR	0.41	0.42	0.01
HuberRegressor	0.33	0.34	0.01
GammaRegressor	0.29	0.3	0.01
TweedieRegressor	0.27	0.28	0.01
RANSACRegressor	0.22	0.23	0.01
OrthogonalMatchingPursuit	0.12	0.13	0.01
PoissonRegressor	-0.01	0	0.01
DummyRegressor	-0.01	0	0.01
ElasticNet	-0.01	0	0.01
Lasso	-0.01	0	0.01
LassoLars	-0.01	0	0.01

QuantileRegressor	-0.12	-0.11	0.01
KernelRidge	-0.78	-0.76	0.01
PassiveAggressiveRegressor	-1.35	-1.32	0.01
SVR	-5.27	-5.18	0.02
MLPRegressor	-9.66	-9.51	0.02
GaussianProcessRegressor	-2563	-2529	0.33

Table S45: ML performance metrics for predicting the volume ($m^3 \cdot kg^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $m^3 \cdot kg^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	69 %	0.004	0	0.006	-0.053
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	69 %	0.004	0	0.006	-0.053
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	67 %	0.004	0	0.006	-0.007
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	67 %	0.004	0	0.006	-0.007
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	57 %	0.003	0	0.005	0.339
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	57 %	0.003	0	0.005	0.34
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	52 %	0.003	0	0.005	0.406
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	52 %	0.003	0	0.005	0.407
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	66 %	0.004	0	0.006	-0.051
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	66 %	0.004	0	0.006	-0.052
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	64 %	0.004	0	0.006	-0.004
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	63 %	0.004	0	0.006	-0.004
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	56 %	0.003	0	0.005	0.34
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	55 %	0.003	0	0.005	0.34
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	49 %	0.003	0	0.005	0.409
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	49 %	0.003	0	0.005	0.41
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	14 %	0.001	0	0.003	0.673
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	14 %	0.001	0	0.003	0.689
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	0.001	0	0.001	0.945
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	7 %	0.001	0	0.001	0.959
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	10 %	0.001	0	0.002	0.859
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	9 %	0.001	0	0.002	0.876
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0	0	0.001	0.971
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	3 %	0	0	0.001	0.988
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	8 %	0.001	0	0.001	0.962
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	7 %	0.001	0	0.001	0.979
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	0	0	0.001	0.973
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	4 %	0	0	0.001	0.99
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	82 %	0.005	0	0.008	-0.654
Exp x NIST	1 %	0	0	0.001	0.983

NIST x Model	82 %	0.005	0	0.008	-0.649
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	237 %	0.013	0.003	0.05	-70.441
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	232 %	0.013	0.003	0.05	-70.381
======== NuSVR_ - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	26 %	0.002	0	0.003	0.682
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	26 %	0.002	0	0.003	0.688
======== NuSVR_ - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	21 %	0.002	0	0.003	0.762
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	21 %	0.002	0	0.003	0.771
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	9 %	0.001	0	0.002	0.919
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	8 %	0.001	0	0.001	0.938
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0	0	0.001	0.965
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	3 %	0	0	0.001	0.982
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	43 %	0.003	0	0.004	0.557
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	43 %	0.003	0	0.004	0.563
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	35 %	0.002	0	0.003	0.701
Exp x NIST	1 %	0	0	0.001	0.983
NIST x Model	34 %	0.002	0	0.003	0.708

S3.8 Enthalpy

Table S46: Evaluation of multiple ML models for the enthalpy (kJ·mol^{-1}) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in kJ·mol^{-1} are presented.

Model	R^2_{adj}	R^2	RMSE
XGBRegressor	1	1	0.12
GradientBoostingRegressor	1	1	0.17
DecisionTreeRegressor	1	1	0.27
ExtraTreesRegressor	0.99	0.99	0.36
ExtraTreeRegressor	0.99	0.99	0.41
RandomForestRegressor	0.98	0.98	0.53
AdaBoostRegressor	0.97	0.98	0.64
BaggingRegressor	0.97	0.97	0.72
KNeighborsRegressor	0.83	0.84	1.62
NuSVR	0.64	0.66	2.37
SVR	0.63	0.65	2.4
HistGradientBoostingRegressor	0.44	0.47	2.95
LGBMRegressor	0.44	0.47	2.96
SGDRegressor	0.08	0.14	3.77
Lars	0.08	0.13	3.78
TransformedTargetRegressor	0.08	0.13	3.78
LinearRegression	0.08	0.13	3.78
Ridge	0.08	0.13	3.78
PoissonRegressor	0.07	0.13	3.8
RidgeCV	0.07	0.13	3.8
BayesianRidge	0.06	0.12	3.82
OrthogonalMatchingPursuit	0.06	0.11	3.83
OrthogonalMatchingPursuitCV	0.06	0.11	3.83
LassoLarsIC	0.04	0.1	3.86
GammaRegressor	0.01	0.07	3.92
TweedieRegressor	0	0.06	3.94
LassoCV	0	0.06	3.95
ElasticNetCV	0	0.06	3.95
LassoLarsCV	0	0.06	3.95
LarsCV	0	0.06	3.95
ElasticNet	-0.05	0.01	4.05
LassoLars	-0.11	-0.05	4.16
DummyRegressor	-0.11	-0.05	4.16
Lasso	-0.11	-0.05	4.16
QuantileRegressor	-0.23	-0.16	4.37
MLPRegressor	-0.81	-0.7	5.3

PassiveAggressiveRegressor	-1.28	-1.15	5.96
LinearSVR	-1.42	-1.28	6.13
HuberRegressor	-1.43	-1.29	6.15
RANSACRegressor	-1.55	-1.4	6.3
KernelRidge	-4.83	-4.49	9.53
GaussianProcessRegressor	-214.7	-202	57.9

Table S47: ML performance metrics for predicting the enthalpy ($kJ \cdot mol^{-1}$) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in $kJ \cdot mol^{-1}$ are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	91 %	2.848	12.845	3.584	-0.152
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	26 %	2.507	9.149	3.025	-0.363
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	75 %	2.631	9.929	3.151	0.109
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	27 %	2.629	10.799	3.286	-0.609
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	69 %	2.746	10.887	3.3	0.023
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	28 %	2.851	13.304	3.647	-0.982
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	74 %	2.624	9.934	3.152	0.109
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	27 %	2.639	11.052	3.324	-0.646
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	95 %	2.719	12.621	3.553	-0.132
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	23 %	2.226	7.022	2.65	-0.046
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	85 %	2.58	10.479	3.237	0.06
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	24 %	2.328	8.075	2.842	-0.203
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	95 %	2.726	12.713	3.566	-0.141
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	23 %	2.237	7.17	2.678	-0.068
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	84 %	2.55	10.258	3.203	0.08
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	24 %	2.316	8.083	2.843	-0.204
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	26 %	0.606	3.359	1.833	0.699
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.572	13.698	3.701	-1.041
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.286	0.127	0.356	0.989
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	14 %	1.703	16.958	4.118	-1.526
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28 %	0.87	3.111	1.764	0.721
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.606	12.657	3.558	-0.885
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0.177	0.304	0.552	0.973
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.634	15.682	3.96	-1.336
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	27 %	0.668	3.444	1.856	0.691
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.515	13.773	3.711	-1.052
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	3 %	0.166	0.071	0.266	0.994
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	14 %	1.689	16.859	4.106	-1.511
======== KNeighbors - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	31 %	0.69	3.629	1.905	0.674
Exp x NIST	122 %	1.683	16.721	4.089	-0.5

NIST x Model	14 %	1.586	12.834	3.582	-0.912
======== KNeighbors - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.422	0.68	0.824	0.939
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	15 %	1.78	15.783	3.973	-1.351
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	94 %	2.657	12.409	3.523	-0.113
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	22 %	2.127	6.66	2.581	0.008
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	88 %	2.766	13.859	3.723	-0.243
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	25 %	2.437	11.242	3.353	-0.675
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	26 %	0.612	3.319	1.822	0.702
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.549	13.427	3.664	-1
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	6 %	0.227	0.27	0.52	0.976
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	13 %	1.637	15.785	3.973	-1.351
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	47 %	1.034	4.05	2.012	0.637
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	12 %	1.381	8.699	2.949	-0.296
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	0.45	0.327	0.572	0.971
Exp x NIST	122 %	1.683	16.721	4.089	-0.5
NIST x Model	14 %	1.698	15.563	3.945	-1.318

S3.9 Viscosity

Table S48: Evaluation of multiple ML models for the Viscosity (µPa·s) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, coefficient of determination (R^2), and root mean squared error (RMSE) in µPa·s are presented.

Model	R^2_{adj}	R^2	RMSE
GaussianProcessRegressor	0.96	0.96	14
GradientBoostingRegressor	0.93	0.94	18.5
LGBMRegressor	0.92	0.92	20.8
ExtraTreesRegressor	0.92	0.92	21
HistGradientBoostingRegressor	0.91	0.91	21.8
XGBRegressor	0.86	0.86	26.8
BaggingRegressor	0.8	0.81	32
AdaBoostRegressor	0.8	0.8	32.3
RandomForestRegressor	0.8	0.8	32.4
ExtraTreeRegressor	0.78	0.78	34.2
DecisionTreeRegressor	0.76	0.77	35.1
PoissonRegressor	0.76	0.77	35.2
KNeighborsRegressor	0.68	0.69	40.6
ElasticNetCV	0.62	0.63	44.4
Ridge	0.62	0.63	44.5
RidgeCV	0.62	0.63	44.5
BayesianRidge	0.62	0.63	44.5
LassoCV	0.62	0.63	44.5
OrthogonalMatchingPursuitCV	0.62	0.63	44.5
TransformedTargetRegressor	0.62	0.63	44.5
LassoLarsCV	0.62	0.63	44.5
LassoLarsIC	0.62	0.63	44.5
LinearRegression	0.62	0.63	44.5
LarsCV	0.62	0.63	44.5
Lars	0.62	0.63	44.5
LassoLars	0.62	0.63	44.5
Lasso	0.62	0.63	44.5
SGDRegressor	0.62	0.62	44.5
MLPRegressor	0.56	0.56	48.1
ElasticNet	0.55	0.56	48.3
OrthogonalMatchingPursuit	0.54	0.55	48.9
LinearSVR	0.47	0.48	52.6
TweedieRegressor	0.46	0.47	52.7
PassiveAggressiveRegressor	0.43	0.44	54.5
HuberRegressor	0.42	0.43	54.8
GammaRegressor	0.4	0.41	55.6

KernelRidge	0.27	0.29	61.4
RANSACRegressor	0.24	0.26	62.6
NuSVR	0.14	0.15	66.9
SVR	0.11	0.13	67.9
DummyRegressor	-0.02	0	72.7
QuantileRegressor	-0.16	-0.14	77.5

Table S49: ML performance metrics for predicting the viscosity (µPa·s) in the supercritical phase. The adjusted coefficient of determination R^2_{adj}, the coefficient of determination (R^2), and the root mean squared error (RMSE) in µPa·s are presented.

======== AdaboostLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	7.148	142.028	11.918	0.166
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	24 %	5.501	66.568	8.159	0.682
======== AdaboostLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33 %	6.268	87.376	9.347	0.487
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	28 %	6.215	82.435	9.079	0.606
======== AdaboostRidge - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	36 %	7.163	142.592	11.941	0.163
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	24 %	5.515	66.813	8.174	0.681
======== AdaboostRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	33 %	6.318	89.12	9.44	0.477
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	28 %	6.279	84.313	9.182	0.597
======== BaggingRegressorLasso - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37 %	7.205	151.624	12.314	0.11
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	24 %	5.516	65.183	8.074	0.688
======== BaggingRegressorLasso - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	31 %	5.947	94.002	9.695	0.448
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	21 %	4.798	47.343	6.881	0.774
======== BaggingRegressorRidge - CV = 10-*fold* ========					

Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	37 %	7.207	151.761	12.319	0.109
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	24 %	5.516	64.984	8.061	0.689
======== BaggingRegressorRidge - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	31 %	5.947	94.021	9.696	0.448
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	21 %	4.792	47.09	6.862	0.775
======== DecisionTree - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	18 %	3.965	122.55	11.07	0.28
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	10 %	3.519	77.196	8.786	0.631
======== DecisionTree - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.197	18.15	4.26	0.893
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	8 %	2.865	85.319	9.237	0.592
======== ExtraTreesRegressor - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	2.415	53.344	7.304	0.687
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	7 %	2.782	71.165	8.436	0.66
======== ExtraTreesRegressor - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.796	6.485	2.547	0.962
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	6 %	2.383	74.552	8.634	0.644
======== GradientBoosting - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	11 %	2.881	60.637	7.787	0.644
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	9 %	3.514	84.762	9.207	0.595
======== GradientBoosting - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	4 %	0.833	7.772	2.788	0.954
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	7 %	2.527	76.654	8.755	0.634
======== LGBM ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	20 %	4.296	95.114	9.753	0.442
Exp x NIST	15 %	2.229	79.406	8.911	0.534

NIST x Model	12 %	3.67	71.478	8.454	0.658
======== NeuralNetwork - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	40 %	8.486	232.236	15.239	-0.364
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	25 %	6.843	123.731	11.123	0.409
======== NeuralNetwork - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	28 %	5.992	117.549	10.842	0.31
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	18 %	4.835	64.115	8.007	0.694
======== RandomForest - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	3.491	92.203	9.602	0.459
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	9 %	3.187	68.366	8.268	0.673
======== RandomForest - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	5 %	1.126	12.784	3.575	0.925
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	7 %	2.527	71.348	8.447	0.659
======== XGB - CV = 10-*fold* ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	32 %	6.137	99.786	9.989	0.414
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	23 %	5.246	65.164	8.072	0.689
======== XGB - CV = LOO ========					
Comparison	MAPE	MAE	MSE	RMSE	R^2
Exp x Model	15 %	3.007	25.179	5.018	0.852
Exp x NIST	15 %	2.229	79.406	8.911	0.534
NIST x Model	16 %	4.246	77.636	8.811	0.629