

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.74×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.29×10^{-1}

Confidence level: 8.93×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Octane

Measured: 8.68×10^{-12}

Predicted: 7.74×10^{-12}

Image not found

2,4-Dimethylpentane

Measured: 5.16×10^{-12}

Predicted: 5.28×10^{-12}

Image not found

Nonane

Measured: 1.02×10^{-11}

Predicted: 8.45×10^{-12}

Image not found

Heptane

Measured: 7.15×10^{-12}

Predicted: 6.52×10^{-12}

Image not found

2,3,4-Trimethylpentane

Measured: 6.99×10^{-12}

Predicted: 5.11×10^{-12}