

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: 2.79e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.19e-01

Confidence level: 8.65e-01

Nearest Neighbors from the Training Set

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(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

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Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12