

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: 7.23e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

Image not found

(Z)-3-Hexen-1-ol

Measured: 1.10e-10

Predicted: 9.25e-11

Image not found

Cyclopentene

Measured: 6.70e-11

Predicted: 6.59e-11

Image not found

Cyclohexene

Measured: 6.77e-11

Predicted: 6.39e-11

Image not found

Norbornylene

Measured: 4.93e-11

Predicted: 5.26e-11

Image not found

Cycloheptene

Measured: 7.40e-11

Predicted: 6.53e-11