

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: 1.48e-12 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.03e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl succinate

Measured: 1.40e-12

Predicted: 1.93e-12

Image not found

Dimethyl glutarate

Measured: 3.30e-12

Predicted: 3.76e-12

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

Image not found

Peroxyacetyl nitrate

Measured: 1.00e-13

Predicted: 9.98e-14

Image not found

2,5-Furandione

Measured: 1.45e-12

Predicted: 2.17e-12