

Octane
111-65-9 | DTXSID0026882

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 11.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.19e-01

Confidence level: 8.73e-01

Nearest Neighbors from the Training Set

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1,2-Ethanediol diacetate

Measured: 14.1

Predicted: 8.89e-02

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3-Methylbutyl 3-methylbutanoate

Measured: 18.4

Predicted: 7.87e-01

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3-Methylbutyl nitrite

Measured: 5.92

Predicted: 1.84

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Methyl dodecanoate

Measured: 4.45

Predicted: 5.38e-03

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Octane

Measured: 17.4

Predicted: 11.4