

Tridecane
629-50-5 | DTXSID6027266

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -4.65 °C

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 9.20e-01

Nearest Neighbors from the Training Set

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Tridecane

Measured: -5.30

Predicted: -4.65

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Tetradecane

Measured: 5.80

Predicted: 3.94

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Dodecane

Measured: -9.60

Predicted: -12.6

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Pentadecane

Measured: 9.90

Predicted: 10.3

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Undecane

Measured: -25.6

Predicted: -14.0