

Dodecane
112-40-3 | DTXSID0026913

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	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.90

Global applicability domain: Inside

Local applicability domain index: 5.54e-01

Confidence level: 5.32e-01

Nearest Neighbors from the Training Set

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Dodecane

Measured: 6.10

Predicted: 5.90

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Tetradecane

Measured: 7.20

Predicted: 7.15

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Decane

Measured: 5.01

Predicted: 5.24

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Cyclohexane, dodecafluoro-

Measured: 2.91

Predicted: 3.19

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Nonane

Measured: 5.65

Predicted: 5.44