

Heptane
142-82-5 | DTXSID6024127

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 42.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.95e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

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Decamethyltetrasiloxane

Measured: 46.0

Predicted: 3.02e-01

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Endosulfan sulfate

Measured: 23.0

Predicted: 2.61e-07

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1-Propene, 3-ethoxy-

Measured: 28.6

Predicted: 160

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1-Methylcyclohexanol

Measured: 34.0

Predicted: 2.05

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1-Bromopentane

Measured: 151

Predicted: 7.15