

Propylbenzene
103-65-1 | DTXSID3042219

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: 2.42 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.39e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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2-Ethylhexyl acrylate

Measured: 3.42

Predicted: 3.32e-01

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Dehydroacetic acid

Measured: 1.69

Predicted: 1.80e-03

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Linolenic acid

Measured: 3.61e-01

Predicted: 5.71e-07

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Furfural

Measured: 4.50

Predicted: 4.06

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4-Vinylcyclohexene

Measured: 9.60

Predicted: 10.4