

4-Phenyltoluene
644-08-6 | DTXSID4047177

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: 17.9 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

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3-Methylbiphenyl

Measured: 4.50

Predicted: 17.9

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4-Phenyltoluene

Measured: 49.5

Predicted: 17.9

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Diphenylmethane

Measured: 25.2

Predicted: 18.5

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Benzene, 1,1'-ethenylidenebis-

Measured: 8.20

Predicted: 24.9