

1-Methyl-2-propylbenzene
1074-17-5 | DTXSID4061466

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: 1.10 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.90e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

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(2-Chlorobenzylidene)propanedinitrile
Measured: 7.39e-01
Predicted: 6.32e-05

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Benzene, 1-chloro-4-ethenyl-
Measured: 2.66
Predicted: 8.25e-01

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Desmetryn
Measured: 9.94e-01
Predicted: 1.39e-06

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1,3-Dimethyl-5-ethylbenzene
Measured: 7.48e-01
Predicted: 9.69e-01

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1-Methyl-3-propylbenzene
Measured: 1.10
Predicted: 1.07