

4-Methylindan
824-22-6 | DTXSID7073931

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: 4.14e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.66e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

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Benzophenone

Measured: 3.68e-01

Predicted: 7.04e-04

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Carbophenothion

Measured: 3.99e-02

Predicted: 4.02e-07

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alpha-d-glucopyranose

Measured: 1.47

Predicted: 3.93e-13

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2,4-Dichloro-1-(chloromethyl)benzene

Measured: 1.10

Predicted: 1.19e-01

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Diethyl pimelate

Measured: 1.00

Predicted: 7.99e-03