

Heptafluorobutyric acid
375-22-4 | DTXSID4059916

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.43

Global applicability domain: Inside

Local applicability domain index: 9.61e-01

Confidence level: 6.25e-01

Nearest Neighbors from the Training Set

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Acetic acid

Measured: 4.31

Predicted: 3.69

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Ethanol

Measured: 3.25

Predicted: 3.05

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Isopropanol

Measured: 3.41

Predicted: 3.68

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1-Propanol

Measured: 3.71

Predicted: 3.75

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Dimethylamine

Measured: 2.00

Predicted: 2.62