

1-Butanol, 2,2,3,3,4,4,4-heptafluoro-
375-01-9 | DTXSID4059914

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: 42.6 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

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Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-

Measured: 33.1

Predicted: 2170

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Ethylene sulfide

Measured: 46.1

Predicted: 166

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1-Decene

Measured: 159

Predicted: 1.31

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Chloral

Measured: 71.3

Predicted: 41.1

[Image not found](#)

Camphor

Measured: 14.7

Predicted: 3.22e-01

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D-Camphor

Measured: 14.7

Predicted: 3.22e-01