

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 91.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.65e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 3,6-dichloro-2-hydroxy-

Measured: 200

Predicted: 49.9

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2,6-Dichlorobenzamide

Measured: 3.39

Predicted: 18.0

[Image not found](#)

Clopyralid

Measured: 36.3

Predicted: 37.7

[Image not found](#)

2-Methoxy-3,5,6-trichloropyridine

Measured: 912

Predicted: 171

[Image not found](#)

Dichlobenil

Measured: 316

Predicted: 328