

Pentadecane
629-62-9 | DTXSID6027268

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: 4130 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.10e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

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4-Nonylphenol

Measured: 6920

Predicted: 1660

Image not found

1-Dodecanol

Measured: 3310

Predicted: 2560

Image not found

Bromoxynil octanoate

Measured: 10000

Predicted: 4120

Image not found

Pentachlor

Measured: 575

Predicted: 365

Image not found

Tribufos

Measured: 5010

Predicted: 4810