

Tridecane
629-50-5 | DTXSID6027266

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: 1610 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.54e-01

Confidence level: 7.05e-01

Nearest Neighbors from the Training Set

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1-Dodecanol

Measured: 3310

Predicted: 2560

Image not found

4-Nonylphenol

Measured: 6920

Predicted: 1660

Image not found

Pentachlor

Measured: 575

Predicted: 365

Image not found

1-Decanol

Measured: 389

Predicted: 347

Image not found

N-Pentyl N-phenylcarbamate

Measured: 407

Predicted: 375