

Hydrogen cyanide
74-90-8 | DTXSID9024148

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: 2.77 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

Image not found

Methanol

Measured: 2.75

Predicted: 2.76

Image not found

Ethyleneimine

Measured: 6.03

Predicted: 4.17

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Acetic acid

Measured: 1.00

Predicted: 2.40

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Ethanol

Measured: 1.58

Predicted: 2.24

Image not found

Thioacetamide

Measured: 6.03

Predicted: 6.43