

4-Aminoazobenzene
60-09-3 | DTXSID6024460

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 337 °C

Global applicability domain: Inside

Local applicability domain index: 3.86e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Aminoazobenzene

Measured: 366

Predicted: 337

[Image not found](#)

3-Methyl-1-phenyl-1H-pyrazol-5-amine

Measured: 333

Predicted: 334

[Image not found](#)

2,4-Dinitroaniline

Measured: 334

Predicted: 330

[Image not found](#)

2,4,5-Trinitrotoluene

Measured: 300

Predicted: 309

[Image not found](#)

2,3,4-Trinitrotoluene

Measured: 301

Predicted: 309