

Diphenylamine
122-39-4 | DTXSID4021975

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: 306 °C

Global applicability domain: Inside

Local applicability domain index: 5.54e-01

Confidence level: 8.61e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diphenylamine

Measured: 302

Predicted: 306

[Image not found](#)

3-Methyl-N-phenylaniline

Measured: 316

Predicted: 318

[Image not found](#)

2-Biphenylamine

Measured: 299

Predicted: 304

[Image not found](#)

4-Biphenylamine

Measured: 302

Predicted: 303

[Image not found](#)

Benzenamine, 3-phenoxy-

Measured: 315

Predicted: 305