

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 54.4 °C

Global applicability domain: Inside

Local applicability domain index: 8.38e-01

Confidence level: 5.90e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diphenylamine

Measured: 52.9

Predicted: 54.4

[Image not found](#)

3-Methyl-N-phenylaniline

Measured: 30.0

Predicted: 51.4

[Image not found](#)

4,4'-Dimethyldiphenylamine

Measured: 79.8

Predicted: 60.6

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2,2'-Diethyldiphenylamine

Measured: 29.0

Predicted: 44.5

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10,11-Dihydro-5H-dibenz[b,f]azepine

Measured: 107

Predicted: 84.2