

6-Quinolinamine, N,N,2-trimethyl-
92-99-9 | DTXSID6059075

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.91e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

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Pentylcyclohexane

Measured: 2.00e-06

Predicted: 6.06e-01

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p-Ethylacetophenone

Measured: 3.92e-04

Predicted: 3.30e-01

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4-Aminoazobenzene

Measured: 7.00e-08

Predicted: 1.49e-06

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1,1':4',1"-Terphenyl

Measured: 6.11e-04

Predicted: 7.62e-06

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Benzoin

Measured: 1.93e-03

Predicted: 3.53e-06

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Benzoin

Measured: 1.93e-03

Predicted: 3.53e-06