

Benzeneethanimidamide, N-phenyl-
7118-59-4 | DTXSID70221381

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: 136 °C

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 3.66e-01

Nearest Neighbors from the Training Set

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3-Amino-9-ethylcarbazole

Measured: 99.0

Predicted: 119

Image not found

Quinoline-2-carbonitrile

Measured: 95.0

Predicted: 89.8

Image not found

Quinoline-3-carbonitrile

Measured: 109

Predicted: 89.8

Image not found

4-cyanoquinoline

Measured: 104

Predicted: 89.8

Image not found

2-Phenylbenzimidazole

Measured: 293

Predicted: 195