

Phenol, 3-methoxy-5-(2-phenylethyl)-
17635-59-5 | DTXSID80170114

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.00e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.18e-01

Confidence level: 4.94e-01

Nearest Neighbors from the Training Set

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Naproxen

Measured: 6.91e-05

Predicted: 8.57e-03

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Hexylparaben

Measured: 1.12e-04

Predicted: 8.87e-03

[Image not found](#)

Pentylparaben

Measured: 1.54e-04

Predicted: 1.40e-02

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3-Amino-3-(naphthalen-1-yl)propanoic acid

Measured: 2.57e-02

Predicted: 1.36e-02

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Heptylparaben

Measured: 8.46e-05

Predicted: 8.31e-04