

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.62e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

Image not found

Haloxypop-etotyl

Measured: 1.28e-05

Predicted: 2.32e-07

Image not found

N-Nitrosodimethylamine

Measured: 1.36e-06

Predicted: 3.96

Image not found

Methyl tridecanoate

Measured: 1.00e-04

Predicted: 1.71e-03

Image not found

Methyl salicylate

Measured: 5.27e-06

Predicted: 4.27e-03

Image not found

Anthracene

Measured: 1.40e-06

Predicted: 2.09e-05