

Ethylbenzene
100-41-4 | DTXSID3020596

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: 5.31 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.15e-01

Confidence level: 8.14e-01

Nearest Neighbors from the Training Set

Image not found

4-Vinylcyclohexene

Measured: 9.60

Predicted: 10.4

Image not found

N-tert-Butyl-2-benzothiazolesulfenamide

Measured: 6.61

Predicted: 2.66e-07

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Dehydroacetic acid

Measured: 1.69

Predicted: 1.80e-03

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Benzene, chloropentafluoro-

Measured: 6.79

Predicted: 24.1

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2-Ethylhexyl acrylate

Measured: 3.42

Predicted: 3.32e-01