

Sulfone, methyl pentafluorophenyl
651-85-4 | DTXSID30215403

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.55

Global applicability domain: Inside

Local applicability domain index: 4.64e-01

Confidence level: 8.69e-01

Nearest Neighbors from the Training Set

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Sulfolane

Measured: 7.08

Predicted: 6.91

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tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

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Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07

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4-Nitroaniline

Measured: 3.98

Predicted: 3.86

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3-Nitroaniline

Measured: 3.02

Predicted: 3.86