

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.74e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.52e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dimethyl glutarate

Measured: 6.94e-03

Predicted: 1.20e-01

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Formanilide

Measured: 2.57

Predicted: 7.22e-04

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Benzene, 1-(1-isocyanato-1-methylethyl)-4-(1-methylethenyl)-

Measured: 1.94e-01

Predicted: 3.05e-03

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Phenol, 4-(1,1-dimethylethyl)-2-methyl-

Measured: 2.59e-01

Predicted: 1.51e-02

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2-Phenylethyl acetate

Measured: 1.94e-01

Predicted: 5.50e-02