

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.75e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.67e-01

Confidence level: 6.01e-01

Nearest Neighbors from the Training Set

Image not found

Methanesulfonyl fluoride

Measured: 3.06e-01

Predicted: 1.68e-01

Image not found

Propane, 2-((1,1-dimethylethyl)sulfonyl)-2-methyl-

Measured: 6.06e-02

Predicted: 3.73e-02

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Benzene, 1-methyl-4-(methylsulfonyl)-

Measured: 1.03e-02

Predicted: 3.51e-02