

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 185 °C

Global applicability domain: Inside

Local applicability domain index: 3.02e-01

Confidence level: 6.98e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pentafluorobenzenesulfonyl
chloride

Measured: 211

Predicted: 186

[Image not found](#)

Pentafluorobenzoyl chloride

Measured: 159

Predicted: 164

[Image not found](#)

2,3,5,6-Tetrafluorobenzaldehyde

Measured: 178

Predicted: 157

[Image not found](#)

Benzoyl chloride, 3-
(trifluoromethyl)-

Measured: 187

Predicted: 181

[Image not found](#)

Pentafluorobenzyl bromide

Measured: 175

Predicted: 164