

1-Methylpyrene
2381-21-7 | DTXSID0025654

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 9.05

Global applicability domain: Inside

Local applicability domain index: 9.74e-01

Confidence level: 4.68e-01

Nearest Neighbors from the Training Set

Image not found

Heptachlor

Measured: 7.64

Predicted: 9.23

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p,p'-DDD

Measured: 10.1

Predicted: 9.39

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1,2,3,4-Tetrachlorodibenzo-p-dioxin

Measured: 9.70

Predicted: 8.59

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2,2',5,5'-Tetrachlorobiphenyl

Measured: 8.47

Predicted: 8.66

Image not found

1,2,3,4,6,7-Hexachloronaphthalene

Measured: 9.58

Predicted: 9.78