

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.03

Global applicability domain: Inside

Local applicability domain index: 5.02e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Fenclofenac

Measured: 4.80

Predicted: 3.59

[Image not found](#)

Triclosan

Measured: 4.76

Predicted: 4.29

[Image not found](#)

3,5-Dichlorodiphenyl ether

Measured: 5.21

Predicted: 3.88

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4,4'-Dichlorodiphenyl ether

Measured: 5.25

Predicted: 3.71