

2-Methylphenanthrene
2531-84-2 | DTXSID1025649

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 24400 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.08e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

Image not found

9-Methylanthracene

Measured: 64600

Predicted: 29700

Image not found

Phenanthrene

Measured: 22400

Predicted: 19900

Image not found

Anthracene

Measured: 20400

Predicted: 19600

Image not found

2-Aminoanthracene

Measured: 28200

Predicted: 24300

Image not found

9-Anthracenemethanol

Measured: 4070

Predicted: 5400