

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 381 °C

Global applicability domain: Inside

Local applicability domain index: 5.40e-01

Confidence level: 7.14e-01

Nearest Neighbors from the Training Set

Image not found

Fluoranthene

Measured: 384

Predicted: 379

Image not found

Pyrene

Measured: 404

Predicted: 379

Image not found

11H-Benzo[a]fluorene

Measured: 405

Predicted: 377

Image not found

4H-

Cyclopenta(def)phenanthrene

Measured: 353

Predicted: 344

Image not found

1-Phenyl-naphthalene

Measured: 334

Predicted: 345