

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 337 °C

Global applicability domain: Inside

Local applicability domain index: 6.08e-01

Confidence level: 9.04e-01

Nearest Neighbors from the Training Set

Image not found

3-Methylphenanthrene

Measured: 350

Predicted: 337

Image not found

Anthracene

Measured: 340

Predicted: 337

Image not found

Phenanthrene

Measured: 340

Predicted: 337

Image not found

Dibenzothiophene

Measured: 333

Predicted: 316

Image not found

3,3'-Dichloro-1,1'-biphenyl

Measured: 320

Predicted: 312