

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 164 °C

Global applicability domain: Inside

Local applicability domain index: 8.68e-01

Confidence level: 5.05e-01

Nearest Neighbors from the Training Set

[Image not found](#)

9-Methylbenz(a)anthracene

Measured: 152

Predicted: 168

[Image not found](#)

Benz(a)anthracene, 3-methyl-

Measured: 157

Predicted: 168

[Image not found](#)

Methylchrysene, 1-

Measured: 257

Predicted: 168

[Image not found](#)

12-Methylbenz[a]anthracene

Measured: 138

Predicted: 168

[Image not found](#)

11-Methylbenzanthracene

Measured: 118

Predicted: 168