

Phenanthrene, trimethyl-
30232-26-9 | DTXSID90184328

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: 145 °C

Global applicability domain: Inside

Local applicability domain index: 9.01e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

Image not found

Retene

Measured: 101

Predicted: 133

Image not found

3,6-Dimethylphenanthrene

Measured: 145

Predicted: 141

Image not found

9,10-Dimethylanthracene

Measured: 183

Predicted: 141

Image not found

Phenanthrene, 9,10-dimethyl-

Measured: 144

Predicted: 141

Image not found

2-Ethylanthracene

Measured: 152

Predicted: 134