

Anisole
100-66-3 | DTXSID4041608

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: -39.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.88e-01

Confidence level: 7.99e-01

Nearest Neighbors from the Training Set

Image not found

Anisole

Measured: -37.5

Predicted: -39.6

Image not found

Benzyl methyl ether

Measured: -52.6

Predicted: -39.7

Image not found

Benzene, ethoxy-

Measured: -29.5

Predicted: -38.7

Image not found

Benzene, 1-methoxy-2-methyl-

Measured: -34.1

Predicted: -38.9

Image not found

3-Methoxytoluene

Measured: -47.0

Predicted: -38.9