

1,3-Dimethyl-4-ethylbenzene
874-41-9 | DTXSID0061246

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: -63.5 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 7.66e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: -62.9

Predicted: -63.5

Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: -66.9

Predicted: -63.5

Image not found

2-Ethyl-p-xylene

Measured: -53.7

Predicted: -63.5

Image not found

1-Ethyl-2,3-dimethylbenzene

Measured: -49.5

Predicted: -63.5

Image not found

1,3-Dimethyl-5-ethylbenzene

Measured: -84.3

Predicted: -63.5