

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1840 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.66e-01

Confidence level: 6.94e-01

Nearest Neighbors from the Training Set

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1,2,4,5-Tetramethylbenzene

Measured: 1320

Predicted: 1510

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2,3,5-Trimethylphenol

Measured: 4070

Predicted: 345

Image not found

Propylbenzene

Measured: 741

Predicted: 859

Image not found

Butylbenzene

Measured: 2450

Predicted: 1580

Image not found

Indan-5-ol

Measured: 2510

Predicted: 653