

Toluene
108-88-3 | DTXSID7021360

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.73

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

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1,3,5-Cycloheptatriene

Measured: 2.63

Predicted: 2.54

Image not found

Ethylbenzene

Measured: 3.15

Predicted: 3.27

Image not found

1,3,5,7-Cyclooctatetraene

Measured: 3.08

Predicted: 2.81

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Benzene, 1,2-difluoro-

Measured: 2.37

Predicted: 2.97