

Tridecane
629-50-5 | DTXSID6027266

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.64×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.37×10^{-1}

Confidence level: 9.05×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Tridecane

Measured: 1.60×10^{-11}

Predicted: 1.64×10^{-11}

Image not found

Tetradecane

Measured: 1.92×10^{-11}

Predicted: 1.90×10^{-11}

Image not found

Dodecane

Measured: 1.42×10^{-11}

Predicted: 1.31×10^{-11}

Image not found

Pentadecane

Measured: 2.22×10^{-11}

Predicted: 2.07×10^{-11}

Image not found

Undecane

Measured: 1.32×10^{-11}

Predicted: 1.05×10^{-11}