

Pentadecane
629-62-9 | DTXSID6027268

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.65e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.21e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found

Tetradecane

Measured: 3.43e-03

Predicted: 1.14e-02

Image not found

Dialifor

Measured: 4.54e-03

Predicted: 1.07e-07

Image not found

Tridecane

Measured: 1.16e-02

Predicted: 6.33e-02

Image not found

Tetradecanoic acid

Measured: 1.43e-03

Predicted: 1.85e-06

Image not found

Pentadecane

Measured: 2.64e-03

Predicted: 3.65e-03