

1-Dodecyl-2,4-dimethylpyridin-1-ium iodide
88477-51-4 | DTXSID00748410

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 5.55e-09 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.57e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found

Pentadecane

Measured: 3.58e-10

Predicted: 1.53e-09

Image not found

Hexadecane

Measured: 3.97e-09

Predicted: 4.12e-09

Image not found

Tetradecane

Measured: 1.97e-08

Predicted: 1.05e-08

Image not found

Decylbenzene

Measured: 1.10e-08

Predicted: 9.66e-08

Image not found

Tridecane

Measured: 2.55e-08

Predicted: 1.55e-08