

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

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 904

Global applicability domain: Outside

Local applicability domain index: 2.90e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Hexadecane

Measured: 5010

Predicted: 3680

[Image not found](#)

Trioctylamine

Measured: 85.1

Predicted: 106

[Image not found](#)

Dodecane

Measured: 240

Predicted: 374

[Image not found](#)

2,6-Dicyclohexylphenol

Measured: 1050

Predicted: 427