

Phenylalanine
150-30-1 | DTXSID9023463

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: 3.31×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.05×10^{-1}

Confidence level: 6.90×10^{-1}

Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35×10^{-11}

Predicted: 2.15×10^{-11}

Image not found

1,4-Benzoquinone

Measured: 4.60×10^{-12}

Predicted: 5.97×10^{-12}

Image not found

(2E)-2-Hexenal

Measured: 4.40×10^{-11}

Predicted: 4.31×10^{-11}