

Alanine, 2-methyl-
62-57-7 | DTXSID0058772

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: 8.24e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 4.72e-01

Nearest Neighbors from the Training Set

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4-Ethoxyaniline

Measured: 7.71e-02

Predicted: 2.72e-02

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2-Methylpropanenitrile

Measured: 4.70e-01

Predicted: 35.5

[Image not found](#)

Carbon dioxide

Measured: 1.00

Predicted: 15000

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Diethyl hexanedioate

Measured: 4.04e-01

Predicted: 4.14e-02

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Diisobutylamine

Measured: 1.25e-04

Predicted: 11.4