

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.66 days

Global applicability domain: Outside

Local applicability domain index: 3.44e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Propylbenzene

Measured: 24.3

Predicted: 4.02

[Image not found](#)

Ethylbenzene

Measured: 120

Predicted: 6.21

[Image not found](#)

Ethylcyclopentane

Measured: 511

Predicted: 8.14

[Image not found](#)

2-Methylhexane

Measured: 12.5

Predicted: 5.54

[Image not found](#)

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95