

Methyl salicylate
119-36-8 | DTXSID5025659

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.84e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

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2-Hydroxypropyl acrylate

Measured: 7.68

Predicted: 5.09

Image not found

Butyl lactate

Measured: 2.74e-01

Predicted: 2.78e-01

Image not found

2-Hydroxyethyl methacrylate

Measured: 7.68e-01

Predicted: 2.04

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Pentyl 2-hydroxypropanoate

Measured: 6.24e-02

Predicted: 1.34e-01