

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.94

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

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Methyl salicylate

Measured: 2.55

Predicted: 1.94

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Benzeneacetic acid, 4-methoxy-

Measured: 1.42

Predicted: 1.77

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Methyl 3-hydroxybenzoate

Measured: 1.89

Predicted: 2.06

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Methylparaben

Measured: 1.96

Predicted: 2.06