

Pyrogallol
87-66-1 | DTXSID6025983

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: 8.46e-01

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 6.59e-01

Nearest Neighbors from the Training Set

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Salicyl alcohol

Measured: 0.73

Predicted: 7.49e-01

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4-Methylcatechol

Measured: 1.37

Predicted: 1.12

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3,4-Dihydroxybenzoic acid

Measured: 0.86

Predicted: 9.42e-01

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1,3,5-Trihydroxybenzene

Measured: 0.16

Predicted: 8.85e-01

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Benzaldehyde, 3,4-dihydroxy-

Measured: 1.09

Predicted: 8.31e-01