

Resorcinol
108-46-3 | DTXSID2021238

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: 4.69e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

Image not found

Tribromoacetic acid

Measured: 6.74e-01

Predicted: 5.34e-01

Image not found

Dibromoacetic acid

Measured: 9.69

Predicted: 4.01

Image not found

6-Hydroxy-4(1H)-pyrimidinone

Measured: 2.23e-02

Predicted: 9.37e-01

Image not found

3-Hydroxybenzyl alcohol

Measured: 5.40e-01

Predicted: 1.00