

Guanidine, (2-benzothiazolyl)-
2582-07-2 | DTXSID20180474

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.14

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.46e-01

Nearest Neighbors from the Training Set

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4-Hydroxybenzoic acid

Measured: 8.08

Predicted: 7.78

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Salicylic acid

Measured: 7.44

Predicted: 7.60

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Phenacetin

Measured: 9.59

Predicted: 9.23

[Image not found](#)

Diphenylamine

Measured: 7.64

Predicted: 8.73

[Image not found](#)

1-Hexadecanol

Measured: 9.90

Predicted: 9.79