

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 75.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 7.29e-01

Nearest Neighbors from the Training Set

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Dimethyl phthalate

Measured: 39.8

Predicted: 59.9

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Diamidafos

Measured: 32.4

Predicted: 34.8

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Urea, (3-chloro-4-methoxyphenyl)-

Measured: 100

Predicted: 47.5

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(3-Methyl-4-bromophenyl)urea

Measured: 234

Predicted: 137

Image not found

[3-(Trifluoromethyl)phenyl]urea

Measured: 95.5

Predicted: 94.0