

Terbutylazine
5915-41-3 | DTXSID4027608

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: 8.43

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.48e-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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1-Octadecanol

Measured: 10.9

Predicted: 10.5

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1-Hexadecanol

Measured: 9.90

Predicted: 9.79

[Image not found](#)

Diphenylamine

Measured: 7.64

Predicted: 8.73