

Acibenzolar-S-methyl
135158-54-2 | DTXSID1032519

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 12.2

Global applicability domain: Inside

Local applicability domain index: 5.05e-01

Confidence level: 5.91e-01

Nearest Neighbors from the Training Set

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O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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2-(Thiocyanomethylthio)benzothiazole

Measured: 209

Predicted: 13.0

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Cyanophos

Measured: 36.3

Predicted: 7.14

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6-Nitrobenzimidazole

Measured: 2.51

Predicted: 3.81