

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.85e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.70e-01

Confidence level: 3.87e-01

Nearest Neighbors from the Training Set

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Acibenzolar-S-methyl

Measured: 3.66e-05

Predicted: 9.85e-05

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2,7,8,9-Tricyclazole

Measured: 8.45e-03

Predicted: 2.09e-04

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Captan

Measured: 1.70e-05

Predicted: 4.23e-05

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Benzthiazuron

Measured: 5.79e-05

Predicted: 1.30e-03

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Bis(ethylxanthogen)

Measured: 1.14e-05

Predicted: 4.06e-05