

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.93e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.26e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

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Quinoxifen

Measured: 3.30e-06

Predicted: 2.19e-08

Image not found

C.I. Disperse Orange 3

Measured: 1.50e-06

Predicted: 6.34e-10

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Butyl ether

Measured: 4.00e-09

Predicted: 8.41

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1-Phenylnonane

Measured: 1.12e-07

Predicted: 4.22e-03

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2,2',4,5'-Tetrachlorobiphenyl

Measured: 2.00e-07

Predicted: 2.93e-05