

4-Aminoacridine
578-07-4 | DTXSID80206487

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: 1.09e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.90e-01

Confidence level: 3.05e-01

Nearest Neighbors from the Training Set

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1-Nitroanthraquinone

Measured: 5.00e-09

Predicted: 9.88e-09

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Fensulfothion

Measured: 5.00e-11

Predicted: 2.64e-05

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Methylcyclopentane

Measured: 9.75e-11

Predicted: 80.1

[Image not found](#)

Tributyl phosphate

Measured: 2.09e-07

Predicted: 2.30e-03

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2,3-Benzofluorene

Measured: 1.35e-04

Predicted: 2.22e-07