

Atrazine

1912-24-9 | DTXSID9020112

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -10.8 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.44e-01

Confidence level: 7.45e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cycloate

Measured: -10.5

Predicted: -10.5

[Image not found](#)

EPTC

Measured: -10.5

Predicted: -10.5

[Image not found](#)

Diethyl sulfate

Measured: -11.7

Predicted: -11.8

[Image not found](#)

Isoproturon

Measured: -10.9

Predicted: -10.5

[Image not found](#)

Triethyl phosphate

Measured: -10.3

Predicted: -10.4