

Sebutylazine
7286-69-3 | DTXSID7058171

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.78e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.39e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

Image not found

Cycloate

Measured: 3.54e-11

Predicted: 2.98e-11

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Isoproturon

Measured: 1.20e-11

Predicted: 3.23e-11

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EPTC

Measured: 3.18e-11

Predicted: 2.83e-11

Image not found

1-Nitro-2-methylnaphthalene

Measured: 8.00e-12

Predicted: 3.49e-11

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11