

Se-(8-Azidoadenosyl)selenomethionine

135608-83-2 | DTXSID70159478

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 314 °C

Global applicability domain: Outside

Local applicability domain index: 5.58e-02

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

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Ametryn

Measured: 345

Predicted: 341

[Image not found](#)

Desmetryn

Measured: 345

Predicted: 341

[Image not found](#)

Tetraethylenepentamine

Measured: 342

Predicted: 339

[Image not found](#)

2,4,6-Tricyano-1,3,5-triazine

Measured: 262

Predicted: 264

[Image not found](#)

Triethylenetetramine

Measured: 267

Predicted: 265