

Cyromazine
66215-27-8 | DTXSID6023999

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

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: 2.44e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.22e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

Image not found

2,4,6-Trimethylpyridine

Measured: 3.59e-10

Predicted: 8.58e-01

Image not found

p,p'-DDE

Measured: 4.46e-11

Predicted: 2.89e-06

Image not found

1-Isobutoxypropan-2-ol

Measured: 7.13e-08

Predicted: 1.69

Image not found

Butylated hydroxytoluene

Measured: 2.00e-10

Predicted: 3.94e-03