

Psicofuranine
1874-54-0 | DTXSID80172052

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: 1.62e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.92e-01

Confidence level: 4.04e-01

Nearest Neighbors from the Training Set

Image not found

1-Isobutoxypropan-2-ol

Measured: 7.13e-08

Predicted: 1.69

Image not found

9,10-Anthracenedione, 1,4-bis(methylamino)-

Measured: 1.80e-08

Predicted: 4.57e-11

Image not found

4-Chloro-3-methylphenol

Measured: 1.50e-12

Predicted: 5.35e-02

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2,4,6-Trimethylpyridine

Measured: 3.59e-10

Predicted: 8.58e-01