

Famotidine
76824-35-6 | DTXSID5023039

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: 1.87e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.47e-01

Confidence level: 4.94e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 1.80e-08

Predicted: 4.57e-11

Image not found

2,4,6-Trimethylpyridine

Measured: 3.59e-10

Predicted: 8.58e-01

Image not found

1-Isobutoxypropan-2-ol

Measured: 7.13e-08

Predicted: 1.69

Image not found

Cloxyfonac [ISO]

Measured: 6.86e-12

Predicted: 3.84e-07